TMP Elite Master Course
Theoretical and Mathematical Physics

LMU LUDWIG-
MAXIMILIANS-
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Master's Thesis

On the Physical Origin of the Lamb Shift

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Meiner Familie und meinen Freunden gewidmet, die mehr für mich getan haben, als ihnen bewusst sein mag.
Danke!

Abstract

Understanding the Lamb shift is one of the milestones of QED and atomic physics. We revisit this central effect from a new angle: after being led to the hypothesis that the Lamb shift may be caused by radiation-like effects, we attempt to construct a quantum-mechanical implementation of the electromagnetic radiation reaction. Upon learning that this appears to give a satisfactory description of at least the linewidths predicted by the Lamb shift, we follow an insight of Dirac and utilize it in a self-field formulation of bound-state QED by Barut. This supports the idea of the decay widths being produced solely by radiation, while the shift of energy levels needs better investigation of how the electromagnetic mass can be explained on a quantum level.

Contents

Introduction

The Lamb shift is one of the milestones of quantum-field-theoretical predictions. It was one of the first phenomena to establish that relativistic quantum physics beyond Dirac's equation exists and it keeps being one of physics' most treasured results, spawning interesting insight into the structure of protons as well as giving precise measurements of the fine-structure constant.

However, we do not fully understand it. Quantum electrodynamics (QED) suggests that the effect is due to the interaction of a propagating electron with the photonic vacuum. This interpretation comes with a grain of salt since the calculations are only possible after a dubious infinite renormalization. Even without this renormalization procedure, we cannot use the diagrams used in QED's S-matrix expansion as representatives of physical reality as they are only terms in a – possibly even divergent – power series.

Still, QED provides phantastic numerical predictions for scattering experiments as they are performed at CERN and for bound-state effects like the anomalous magnetic moment of the electron and, in fact, the Lamb shift. While this certainly makes QED our best approach to effects like the above, its problems are far too often being disregarded as either being only mathematical details or unimportant for the effective theory as which most physicists nowadays understand quantum electrodynamics.

These problems are not all new to QED. One of the worst of them, the ultra-violet divergence of all expressions involving loops, is completely inherited from Maxwell electrodynamics. It is therefore quite surprising that no serious effort has been made to find a "quantum" version of the only completely divergence-free theory of charged particles we know, Wheeler-Feynman electrodynamics.

As tabletop-sized experiments begin to enter the energy range in which a quantum theory of light and matter for finite times becomes important, it is necessary to identify the true physical mechanisms, be it those giving a relativistic quantum mechanics of many particles or those responsible for the quantized electromagnetic field – or, in the spirit of Wheeler and Feynman, those relativistic theories that interact completely without electromagnetic fields.

The situation is somewhat similar to that of the Casimir effect. While the textbook explanation for this phenomenon uses vacuum fluctuations and renormalization

techniques, there are strong reasons to believe that van-der-Waals forces are the true mechanism behind the Casimir effect, see [**Jaf05**].

Jaynes' Bet

The Lamb shift and its explanation using vacuum fluctuations of the photon field, which produce a difference in mass between bound and free particle and even between bound states with different angular momenta has been criticised before. It is quite well-known that Jaynes even placed a bet claiming that he could find a semi-classical description of the Lamb shift, coining the expression *neoclassical physics*. He was able to produce the imaginary part of the Lamb shift, *i.e.* spontaneous emission, but did not quite arrive at a correct description for the energy shift. Nevertheless, his strong objections towards the infinite "subtraction physics" [**Jay90**] of quantum electrodynamics should not be dismissed on grounds of his lost bet – those problems stand and need to be solved.

Purpose of Thesis

It is the task of this work to find out whether it is possible to point out the physical mechanisms behind the Lamb shift.

In doing so, we revisit the problem of introducing radiation into quantum mechanics, study a toy model for a dissipative perturbation to the Hydrogen Hamiltonian and eventually analyse a possible effective theory for bound state relativistic quantum physics of light and matter introduced by Barut.

We arrive at a satisfactory explanation of the imaginary part of the Lamb shift: it is produced entirely by radiation effects. The real part, however, cannot be fully accounted for, but we at least pinpoint it in a mass term introduced by Dirac.

Organisation of Thesis

In chapter 1, we give a short summary of the problem of radiation reaction in classical physics, introducing Wheeler-Feynman electrodynamics as a possible way to get rid of divergences on the classical level when describing radiation of point charges. After that, the Lamb shift is explained in chapter 2, were we also revisit Bethe's original calculation and include a derivation using time-dependent perturbation theory. Other derivations are also explained with their respective implications and problems mentioned. The core of our work and the original part follow in chapters 3 and 4. In the former, we try to include a radiation reaction into quantum mechanics via different approaches, finally trying to arrive at the Lamb shift. This hints at only the imaginary part of this shift being produced by radiation. The latter chapter then gives a brief introduction to Barut's self-field QED which we utilize to show that the Lamb shift follows exactly the

splitting introduced by Dirac to isolate radiation reaction from a renormalization effect connected to the electromagnetic mass of the electron.

A Note on Terminology

Historically, the term Lamb shift has been used mostly to denote the real part of the effect we are studying which is responsible for the shift of energy levels. Its imaginary part, producing a line width, was not usually referred to as Lamb shift. However, since these two phenomena can be understood as one $\mathbb{C}$-valued effect, we shall call the entire effect Lamb shift and specify with real or imaginary part, respectively.

CHAPTER 1

Radiation Reaction

The problem of accelerated point charges yields insurmountable difficulties in Maxwell-Lorentz electrodynamics, as the Lorentz force diverges at the position of the accelerated charge – as does the $1/r^2$ Coulomb field. It is, however, necessary to allow self-interactions of charged particles to account for radiation phenomena. The only way known to calculate these radiation effects convincingly is to smear out all charges to little balls, which leads to the radiation force expression of Lorentz and Abraham[1]

$$\boldsymbol{F}_{\mathrm{rad}} = \frac{2}{3}\frac{q^2}{c^3}\dddot{\boldsymbol{x}}, \tag{1.1}$$

where q is the charge of the particle, c the speed of light and we are using CGS units. This force is connected to and consistent with the Larmor formula for radiated energy by an accelerated charge

$$P_{\mathrm{rad}} = \frac{2}{3}\frac{q^2}{c^3}\left|\dot{\boldsymbol{x}}\right|^2. \tag{1.2}$$

The method of smearing out all charges is insofar insatisfactory as it presents new problems itself: the famous 4/3 problem, related to the fact that the ansatz still produces a divergent part which has to be included in the mass term; furthermore the question of why an electron should have a complex inner structure which matters for a theory incapable of probing this structure (and why this structure is then not found in quantum physics). A macroscopic theory like that of electromagnetism should really be able to model an electron as a simple point particle, regardless of one's personal view whether elementary particles are indeed point-like.

The relativistic generalization of equation (1.1) was found by Dirac in an ingenious paper [**Dir38**], where he employed mass renormalization techniques to arrive at

$$\mathsf{F}_{\mathrm{rad}} = \frac{2}{3}\frac{q^2}{c^3}\left(\dddot{\mathsf{x}} + \left(\ddot{\mathsf{x}}\cdot\dddot{\mathsf{x}}\right)\dot{\mathsf{x}}\right), \tag{1.3}$$

[1] [**Jac13**] gives a good overview over the entire range of questions in classical electrodynamics we consider here and contains a rich bibliography. Depending on taste, the exposition in [**FLS05**] excellently explains many of the problems.

here given in four-vectorial form (note the difference between $\boldsymbol{x} \in \mathbb{R}^3$ and $\mathsf{x} \in \mathbb{R}^{3+1}$, also, in relativistic notation, a dot over a quantity means derivative with respect to proper time along the trajectory).

The problem of divergent forces on point particles sometimes is taken to be not too severe, as "Maxwell electrodynamics is only the effective theory of quantum electrodynamics at low energies"[2]. Now, if QED repaired these divergences, one could accept such a statement. Unfortunately, these problems reappear similarly in QED in the guise of UV divergences[3], accompanied by the less severe IR divergences and the devastating Landau pole.

In order to make progress towards a well-defined quantum theory of light and matter, it seems necessary to find a never-divergent classical theory of electromagnetism first. The most promising candidate is Wheeler-Feynman electrodynamics (WFE), introduced in [**WF49**] building upon previous ideas by Fokker, Tetrode, Schwarzschild and even Gauß. In one sentence, Wheeler-Feynman electrodynamics is the theory of directly interacting charged particles, there are no fields in the theory. In fact, these particles interact exactly when their Minkowski distance is lightlike and never with themselves, and without any fields. Furthermore, the theory is completely symmetric in time, the "true" interaction being half of the sum of retarded and advanced actions, which in turn are given by stand-in quantities mathematically equivalent to the Liénard-Wiechert fields of ordinary electrodynamics. This has a couple of consequences:

- A particle alone in the universe never feels any electromagnetic forces. To emphasize this fact: there is no self-interaction in Wheeler-Feynman electrodynamics.
- Interactions between two particles generally cascade along the entire trajectories of the particles, making it extremely hard to find a solution theory of Wheeler-Feynman electrodynamics, see [**BDD13**].
- Since radiation always carries energy away from an accelerated charge, this irreversible effect (at least macroscopically) defines an arrow of time which needs explaining in a completely time-symmetric theory.

Somewhat surprisingly, WFE is able to predict radiation effects, even though there is no self-interaction. Boltzmann introduced the correct way to treat emergent irreversibility from a reversible theory: "special", or better atypical, initial conditions typically exhibit irreversible behaviour. Think of the old simile of the falling and breaking glass, where the atypicality of the initial conditions lies in the special arrangement of molecules

[2]This is at least taught in usual QED courses.

[3]These are said to be less of a problem than the $1/r$-divergences of classical electromagnetism, but still they are severe as they need to be repaired by hand in each term of QED's perturbation series.

to form the glass (and also its initial velocity and position on a table etc.) — Wheeler and Feynman argue in [**WF45**] that a distribution of charged particles acting as an "absorber"[4] allows for radiation effects of accelerated charges by this very reasoning.

Unfortunately, Feynman and others after him have failed so far to formulate a quantum mechanical version of Wheeler-Feynman electrodynamics. In fact, Feynman's famous thesis [**Fey05**] introducing the path integral was spawned mainly by the attempt to quantise WFE, as he addresses in his Nobel lecture [**Fey65**].

In mathematical terms, Wheeler-Feynman electrodynamics is defined by an action principle for N particles:

$$S = -\sum_{i=1}^{N} \left\{ m_i c \int \sqrt{(\dot{\mathsf{z}}_i)^2}\, \mathrm{d}\tau_i + \frac{1}{2} \sum_{j \neq i} \frac{q_i q_j}{c} \iint \delta^{(4)}\Big((\mathsf{z}_i - \mathsf{z}_j)^2\Big)\, \dot{\mathsf{z}}_i \cdot \dot{\mathsf{z}}_j \, \mathrm{d}\tau_i \mathrm{d}\tau_j \right\}, \quad (1.4)$$

where τ_i is proper time along the trajectory $\mathsf{z}_i(\tau_i)$ of the i-th particle, q_i its charge, and the squares and "$\cdot$"-scalar products are Minkowskian.

The formal Euler-Lagrange equations of motion for this action look exactly like the Lorentz forces from usual electrodynamics, but with excluded self-interaction, and the field strength tensor is replaced by one-half the sum of the retarded and the advanced fields:

$$m_i \ddot{z}_i^{\mu}(\tau_i) = q_i \sum_{j \neq i} \frac{1}{2} \left\{ F_j^{\mathrm{ret}} + F_j^{\mathrm{adv}} \right\}^{\mu\nu} (\mathsf{z}_i(\tau_i))\, (\dot{z}_i)_{\nu}(\tau_i)\,, \quad (1.5)$$

where

$$\left(F_j^{\mathrm{ret/adv}}\right)^{\mu\nu}(\mathsf{z}) = \frac{\partial \left(A_j^{\mathrm{ret/adv}}\right)^{\nu}}{\partial z^{\mu}}(\mathsf{z}) - \frac{\partial \left(A_j^{\mathrm{ret/adv}}\right)^{\mu}}{\partial z^{\nu}}(\mathsf{z})\,,$$

and the $\mathsf{A}^{\mathrm{ret/adv}}$ are formally equivalent to the retarded/advanced Liénard-Wiechert potentials.

Unfortunately, the completely time-symmetric nature of WFE requires the analysis of delay-type differential equations, where the force on one particle is given by retarded and advanced actions of all other particles *and vice versa*. Thus, we have to know very much about the global trajectories to compute the acceleration of a test charge at a given moment, see figure 1. Of course, to be at the same level as ordinary Maxwell-Lorentz theory, one prescribes the trajectories of the "source" particles and uses them to find that of a test charge.

[4]The notion "absorber" might imply that there is something special about these particles. However, as is argued in [**BDDH14**], any sufficiently well-behaved distribution of charges will do. If one is so inclined, a possible candidate could be the Dirac sea, but we shall not touch upon this topic here.

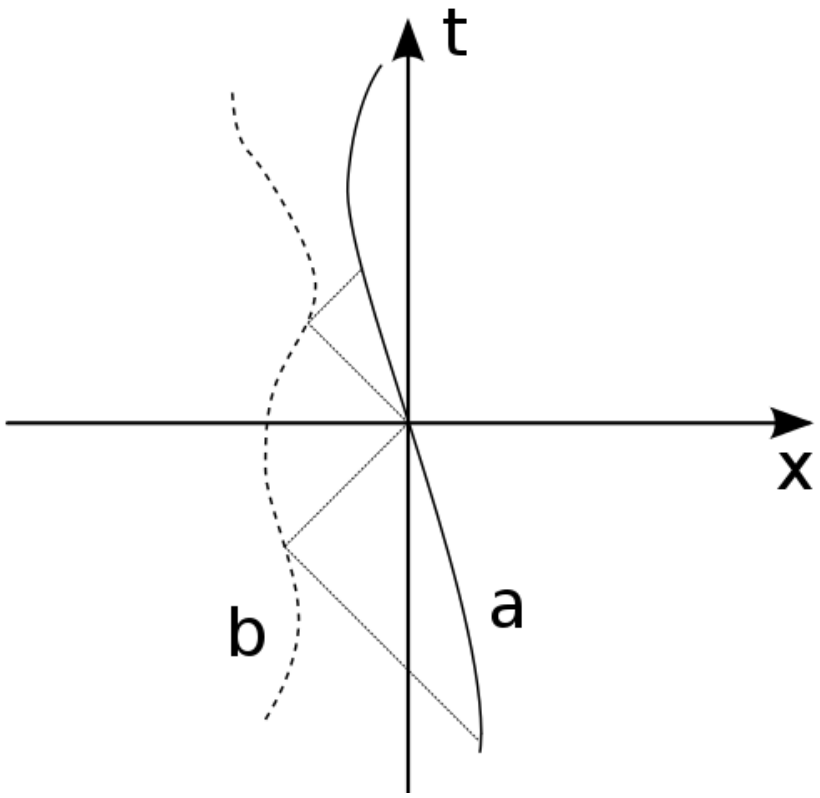


FIGURE 1. Interaction between two charges in Wheeler-Feynman electrodynamics. The dotted lines represent interactions between particles a (full line) and b (dashed line). At a given moment, the actions cascade down the entire trajectories of a and b. We drew only a few of the interactions.

Dirac showed in [**Dir38**] that the radiation field of an accelerated charge is given by $\mathsf{F}_{\mathrm{rad}}(\mathsf{z}) = 1/2\left(\mathsf{F}^{\mathrm{ret}}(\mathsf{z}) - \mathsf{F}^{\mathrm{adv}}(\mathsf{z})\right)$, but had to perform an infinite mass renormalization along the way, where he included a divergent term $1/2\left(\mathsf{F}^{\mathrm{ret}}(\mathsf{z}) + \mathsf{F}^{\mathrm{adv}}(\mathsf{z})\right)$ into the mass of the electron. We will later find this split again, see chapter 4.

The article [**WF45**] is dedicated to arrive at this very expression for the radiation but manages to do so via several different derivations, none of which needed renormalization but instead just the absorber. In essence, Wheeler-Feynman show that while radiation reaction or equivalently self interaction is produced by the accelerated particle's $\mathsf{F}_{\mathrm{rad}}$, the true "field" produced by that particle is $\mathsf{F}_{\mathrm{mass}}(\mathsf{z}) := 1/2\left(\mathsf{F}^{\mathrm{ret}}(\mathsf{z}) + \mathsf{F}^{\mathrm{adv}}(\mathsf{z})\right)$ and thus by superposition a particle in the vicinity of the accelerated charge feels only the retarded field of the latter. The $\mathsf{F}_{\mathrm{mass}}$ however diverges along the trajectory of the point particle.

In conclusion, Maxwell-Lorentz electrodynamics of point particles is just not a well-defined theory and passes its shortcomings on to QED. Wheeler-Feynman electrodynamics on the other hand provides us with such a well-defined theory and is capable of reproducing all established results from ordinary electrodynamics without divergences. This comes at the cost of it being a highly non-trivial theory since its equations are impenetrable for usual mathematical methods when it comes to abstract but in this case essential questions like existence and uniqueness of dynamics.

CHAPTER 2

The Lamb Shift

The inclusion of ever smaller relativistic effects into the Hamiltonian of the Hydrogen atom and the eventual discovery of Dirac's equation lead to an extremely precise theoretical apparatus to describe atomic spectra. Mathematically speaking, additional effects like relativistic mass correction, spin-orbit coupling, fine- and hyperfine-structure terms lifted a lot of the degeneracies present in Schrödinger quantum mechanics.

It was all the more surprising that Lamb and Retherford found a split between energy levels which was unaccounted for in Dirac's relativistic quantum mechanics, see [**LR47**], which was later dubbed Lamb shift. This shift lifts the degeneracy between the $2s_{1/2}$ and $2p_{1/2}$ states of Hydrogen by about 1057 MHz. Less often one learns about the imaginary part of the Lamb shift, which is not to be found in Bethe's original derivation, but which nevertheless exists and is responsible for (part of) the line widths of decays into lower energy states. The exact mechanism is, however, unclear. Hans Bethe provided the first theoretical approach utilizing the then not yet fully developed quantum theory of fields, where after a mass renormalization a logarithmically divergent expression for the Lamb shift was found. A cutoff at mc^2, where m is the electron mass, gave an excellent numerical agreement with Lamb and Retherford's experiment, [**Bet47**].

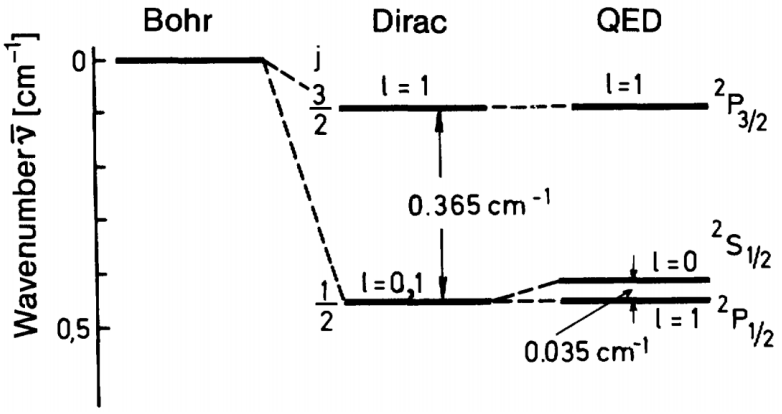


FIGURE 1. The Lamb shift. Taken from [**HH05**].

Bethe's student Dyson, alongside Weisskopf and other physicists, later provided a fully relativistic calculation which improved the numerical accuracy even further, [**Dys11**].

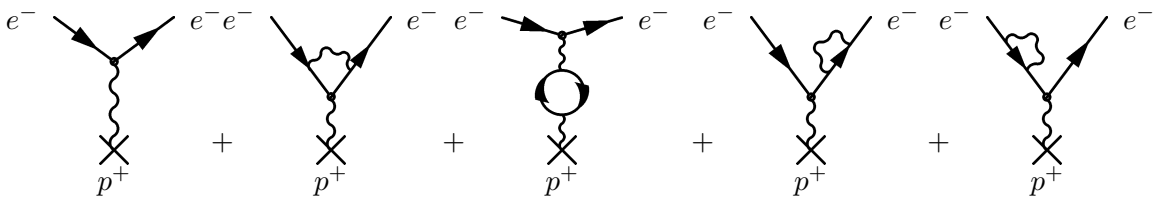
In a more modern language, the Lamb shift is calculated using Quantum Electrodynamics. Even though this formalism essentially only describes scattering experiments due to its crucial need for asymptotic states, the bound-state situation for Hydrogen is actually possible to treat with usual QED methods. It should be stressed that these methods consist to a fair part of recipes to cure the abundance of infinities.

The significance of the Lamb shift can hardly be overestimated. Physics' most accurate measurements are performed measuring the Lamb shift or the connected $g-2$ – anomalous magnetic moment of the electron. Using muons instead of electrons put to question what we know about the proton. And also it is one of the first effects to be successfully described by quantum field theory, thus strengthening its standing as a useful formalism.

In what follows, we will quickly go over different derivations of the Lamb shift from the literature. As those are fairly standard, we shall skip the calculations and just point out essential features of each of the approaches.

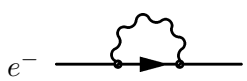
2.1. QED Treatment of the Lamb Shift

To first loop order, there are five Feynman diagrams for the Coulomb problem:



Dirac	Vertex Correction	Vacuum Polarisation	Self Interaction	Self Interaction

Relevant for the Lamb shift are the last two, so essentially the following type of diagram:



This is called a propagator correction and can be evaluated using what are now standard techniques, see [**Wei05**].

We don't want to repeat the (long) full QED calculation of the Lamb shift here, as it can be found in standard textbooks like [**Wei05**] or [**LL91**]. However, we shall outline the central steps in the

2.1.1. Essentials of the QED Treatment.

- We recognize that the usual perturbative treatment breaks down when we consider bound states, since neither the structural properties of atomic states nor the energies involved can be represented in such an ansatz. Instead, it can be shown that the correct QED-propagator for these effects is then a solution to Dirac's equation with the binding potential.
- The relevant Feynman diagram, as shown above, is then extracted. The associated integral diverges, so we need to handle this divergence. Usually what one does is to include counter diagrams which essentially renormalise the integrals. Most often the integrals need to be regularized before they can even be computed. All of this seems very fishy, and even though there are more or less rigorous mathematical arguments that every such divergent diagram can be renormalised (see [**Sch95**][1]), the appearance of divergent expressions should be a boldface and underlined warning that something in our treatment is wrong.
- After renormalization, the integrals can be solved and we find numerical expressions in the expectation value of Hydrogen wave functions (for the Dirac equation) which include both a real and an imaginary part. The real part is what is usually called Lamb shift and rises the energy of s states from their respective p states, thus the degeneracy from Dirac theory disappears. The imaginary part on the other hand contributes to decay widths of the states into lower-energy states. Of course, all numbers are extremely well verified by experiment.
- A true physical mechanism cannot be given because of the extremely doubtworthy nature of all relevant calculations, but one would argue that in this language the Lamb shift comes from *a difference in propagation between free and bound electrons* without really clearing up how this difference comes about.

[1]Here we could dwell a while. There is an approach to QFT by Epstein and Glaser called *causal distribution theory* where the infinities of QED are removed not on the functional/integrals level but on that of distributions. Since all creation and annihilation operators in QED are in fact distributions which usually are completely mistreated by physicists, the hope would be that the divergent integrals of QED stem from improper usage of distributions. This is, however, not the case and the trick to "split" causal distributions is just the same renormalization/regularization on a lower level. Noteworthy for us might be, however, that in this setting one sees a bit more clearly what the relevant physical objects are and finds retarded and advanced distributions, just as one might expect from our line of reasoning.

To summarize, the QED treatment, while extremely precise, veils a lot of the underlying physics – only calling a diagram self energy does not make it a self energy term, especially if the diagram is only a representation of a divergent integral in a possibly non-convergent perturbation series. Taking these diagrams as pictorial representations of physical reality is clearly not a sensible standpoint, but then one should explain in more detail what the physical processes responsible for certain phenomena are. We probably need not talk anymore about the problems at which the ubiquitous divergences hint – at the very least, they make a clear physical picture of the situation impossible.

We shall now go back historically and look at Bethe's original derivation as well as Welton's, both of which tell a much better story about the processes behind the Lamb shift.

2.2. Bethe's Treatment of the Lamb Shift

In an article which is commonly referred to as one of the breakthroughs for quantum field theory, Bethe performed an almost back-of-the-envelope calculation of the Lamb shift. Historically it is remarkable that he completely worked it out on the train ride back from the Shelter Island conference where Lamb's finding was presented and discussed. Essentially, this ansatz is the low-energy (*i.e.* non-relativistic) part of the modern treatment with some subtle differences. We shall quickly revisit Bethe's calculation and leading up to it, the time-dependent perturbation theory necessary to arrive at equation (1) of Bethe's paper [**Bet47**].

2.2.1. An Overview of Bethe's Lamb Shift Calculation. In what follows, we will always use uppercase greek letters like Ψ to represent a state consisting of an electron state ψ and a photonic state, which we never explicitly write out. We start out at the QED Hamiltonian for a hydrogen atom, as usual put $k := |\boldsymbol{k}|$, and use the Dirac current $j^\mu = \mathrm{i}e\overline{\psi}\gamma^\mu\psi$:

$$H = \underbrace{\gamma^0 mc^2 - \mathrm{i}\hbar c\gamma^0\gamma^i\partial_i + V(r)}_{H_A} + \underbrace{\hbar c\int k a_k^{*\mu} a_{k\mu}\,\mathrm{d}^3k}_{H_M} \underbrace{-\frac{1}{c}\int j^\mu(\boldsymbol{x})\,A_\mu(\boldsymbol{x})\,\mathrm{d}^3x}_{H_I}. \tag{2.1}$$

This Hamiltonian satisfies

$$\mathrm{i}\hbar\partial_t\Psi = H\Psi,$$

where we keep in mind that the Dirac current is already bilinear in ψ. The labels of the different terms in the Hamiltonian stand for "Atomic", "Maxwell", and "Interaction", respectively.

It is convenient to work in the interaction picture, thus, let us define

$$\Phi(t) := \mathrm{e}^{\mathrm{i}t(H_A+H_M)/\hbar}\Psi(t)\,, \tag{2.2}$$

which evolves only due to the interaction part of the Hamiltonian in the interaction picture:

$$\mathrm{i}\hbar\partial_t\Phi(t) = H_I(t)\,\Phi(t)\,, \tag{2.3}$$

where

$$H_I(t) = \mathrm{e}^{\mathrm{i}(H_A+H_M)t/\hbar}H_I\mathrm{e}^{-\mathrm{i}(H_A+H_M)t/\hbar}.$$

With these objects at hand, we delve into time-dependent perturbation theory, following closely Dyson's book [**Dys11**].

The setup is as follows: We take the atom to be in a state ϕ_n at time $t = 0$, where n represents not only the main quantum number but is a shorthand for all Dirac quantum numbers. That state's energy is E_n. The photon field at $t = 0$ is assumed to be the vacuum state Ω, and thus $\Phi(t = 0) = \phi_n \otimes \Omega = \Phi_n$. The problem at hand suggests that we calculate the probability of finding the atom in state ϕ_n without any photons present after a long time t, $\langle\Phi_n, \Phi(t)\rangle$, where the scalar product is that of $Ł^2 \otimes \mathcal{F}$, the spin space of square integrable Dirac wavefunctions tensored with the Fock space of photonic states.

We assume that the state of the system at time t is given by a time-dependent superposition of all eigenstates as follows:

$$\Phi(t) = \sum_m a_m(t)\,\Phi_m(t)\,. \tag{2.4}$$

Since interactions involving more than one photon are extremely rare, our perturbation stops at the one-photon level and we get an approximate solution for equation (2.3) by

$$\Phi(t) = \left(1 - \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t} H_I\big(t'\big)\;\mathrm{d}t'\right)\Phi_n.$$

However, our perturbation should respect not only that single-photon effects are the most prominent, but also that after large times, the atomic state will have changed due to radiation. To accomodate this fact, we include *ad-hoc* the expansion parameter $a_n(t)$, which encodes "how much" of state n is still present after a time t, and write:

$$\Phi(t) = \left(1 - \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t} H_I\big(t'\big)\;\mathrm{d}t'\right)a_n(t)\,\Phi_n. \tag{2.5}$$

By our ansatz in eq. (2.4),

$$\langle \Phi_n, \Phi(t) \rangle = a_n(t)\,,$$

and we can find a differential equation for $a_n(t)$ by

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} a_n(t) &= \frac{\mathrm{d}}{\mathrm{d}t} \langle \Phi_n, \Phi(t) \rangle \\ &= -\frac{\mathrm{i}}{\hbar} \langle \Phi, H_I(t)\, \Phi(t) \rangle\end{aligned}$$

which is by above approximation given as

$$\begin{aligned}&= -\frac{\mathrm{i}}{\hbar} \langle \Phi, H_I(t) \left(1 - \frac{\mathrm{i}}{\hbar} \int_{-\infty}^{t} H_I\big(t'\big)\, \mathrm{d}t' \right) a_n(t)\, \Phi_n \rangle \\ &= -\frac{\mathrm{i}}{\hbar} \langle \Phi, \left(H_I(t) - \frac{\mathrm{i}}{\hbar} \int_{-\infty}^{t} H_I(t)\, H_I\big(t'\big)\, \mathrm{d}t' \right) a_n(t)\, \Phi_n \rangle.\end{aligned}$$

Since the photonic part of our state Φ_n is the vacuum, the first term in the parentheses vanishes by it having zero vacuum expectation value and thus

$$\begin{aligned}\frac{1}{a_n(t)} \frac{\mathrm{d}}{\mathrm{d}t} a_n(t) &= -\frac{1}{\hbar^2} \int_{-\infty}^{t} \langle \Phi_n, H_I(t)\, H_I\big(t'\big)\, \Phi_n \rangle\, \mathrm{d}t' \\ &= -\frac{1}{\hbar^2} \int_{-\infty}^{t} \langle A_\mu(\boldsymbol{x}, t)\, A_\nu\big(\boldsymbol{x}', t'\big) \rangle_\Omega \langle j^\mu(\boldsymbol{x}, t)\, j^\nu\big(\boldsymbol{x}', t'\big) \rangle_{\phi_n}\, \mathrm{d}t'.\end{aligned}$$

The vacuum expectation value of the fields is well known to be

$$\langle A_\mu(\mathsf{x})\, A_\nu\big(\mathsf{x}'\big) \rangle_\Omega = \mathrm{i}\hbar c D_{\mathrm{ret}}\big(\mathsf{x} - \mathsf{x}'\big)\, \delta_{\mu\nu},$$

D_{ret} being the retarded propagator, and with the definition (keeping in mind that ϕ is a Dirac wavefunction)

$$T^\mu_{mn}(\boldsymbol{k}) := \langle \phi_m, \int_{\mathbb{R}^3} j^\mu(\boldsymbol{x})\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\, \mathrm{d}^3x\ \phi_n \rangle$$

we find after some straightforward calculations where we used the Sokhotski-Plemelj theorem (see (A.1) in the appendix):

$$\frac{1}{a_n(t)} \frac{\mathrm{d}}{\mathrm{d}t} a_n(t) = \tag{2.6}$$

$$= -\frac{1}{16\pi^3 c} \int \sum_m |T_{nm}(\boldsymbol{k})|^2 \left(\pi\delta(E_m - E_n + \hbar c k) - \mathsf{P.V.} \frac{\mathrm{i}}{E_m - E_n + \hbar c k} \right) \frac{\mathrm{d}^3 k}{k}. \tag{2.7}$$

Obviously, $a_n(t)$ is then given by an exponential function, which we set up as

$$a_n(t) = \exp\left(-\frac{1}{2}\Gamma_n t - \frac{\mathrm{i}}{\hbar}\Delta E_n t\right),$$

because then the energy of state Φ_n will be shifted by ΔE_n and the state decays with $|a_n(t)|^2 = \mathrm{e}^{-\Gamma_n t}$.

The expressions for ΔE_n and Γ_n are read off of equation (2.7):

$$\Gamma_n = \frac{1}{8\pi^2 c}\int \sum_m |T_{nm}(\boldsymbol{k})|^2\, \pi\delta(E_m - E_n + \hbar c k)\, \frac{\mathrm{d}^3 k}{k} \tag{2.8}$$

$$\Delta E_n = -\frac{1}{16\pi^3 c}\int \sum_m |T_{nm}(\boldsymbol{k})|^2\, \mathsf{P.V.}\frac{1}{E_m - E_n + \hbar c k}\, \frac{\mathrm{d}^3 k}{k}. \tag{2.9}$$

For Bethe's calculation, we approximate equation (2.9) for the nonrelativistic case, which entails the dipole approximation for the current and integrating out the angular part and using the Schrödinger current instead of that from Dirac theory, *i.e.* $\boldsymbol{j}^{\psi} = 1/(2m)\,(\psi^*\boldsymbol{p}\psi - \psi\boldsymbol{p}\psi^*)$. Then this energy shift becomes equation (1) from Bethe's paper,

$$\Delta E_n = -\frac{2}{3\pi}\frac{e^2\hbar}{m^2 c}\int_0^\infty k \sum_m \frac{|\boldsymbol{p}_{mn}|^2}{E_m - E_n + \hbar c k}\,\mathrm{d}k, \tag{2.10}$$

with $\boldsymbol{p}_{mn} = \langle \psi_m, \boldsymbol{p}\,\psi_n\rangle$ being the mn-matrix element of the nonrelativistic momentum operator between – now – Schrödinger eigenstates.

2.2.2. Mass Renormalization. This expression diverges, and this is where renormalization comes in. Bethe argues in [**Bet47**] that we should subtract from equation (2.10) the analogue for a free particle, which is given by

$$\begin{aligned}\Delta E_{\text{free}} &= -\frac{2}{3\pi}\frac{e^2\hbar}{m^2 c}\int_0^\infty k\frac{|\boldsymbol{p}|^2}{\hbar c k}\,\mathrm{d}k \\ &= -\frac{2e^2}{3\pi m^2 c^2}\int_0^\infty |\boldsymbol{p}|^2\,\mathrm{d}k.\end{aligned}$$

Similar to what happens in the Abraham-Lorentz equation or Dirac's relativistic computation of radiation reaction, we identify this term as a part of the kinetic energy due to its dependence on $\boldsymbol{p}^2$ and reason as follows:

The kinetic energy of the electron gives rise to measurements of its mass, call it M. However, if we embed the electron in the electromagnetic field, there is a shift in its

energy:

$$\begin{aligned}\frac{1}{2}Mv^2 &= \frac{1}{2}\mu v^2 - \frac{2e^2}{3\pi c^2}v^2\int_0^\infty \mathrm{d}k \\ &= \frac{1}{2}v^2\left(\mu - \frac{4e^2}{3\pi c^2}\int_0^\infty \mathrm{d}k\right)\end{aligned}$$

This means that the *actual* mass of the electron μ must tend to infinity to properly include the diverging integral. But then, the free effect is already included in the mass and thus has to be subtracted from our treatment. Hence, the actual, renormalized energy shift is given by

$$\Delta E_n^{\mathrm{ren}} = \Delta E_n - \Delta E_{\mathrm{free}} \tag{2.11}$$

$$= \frac{2e^2}{3\pi m^2 c^2}\int_0^\infty \sum_m \frac{(E_m - E_n)\,|\boldsymbol{p}_{mn}|^2}{E_m - E_n + \hbar ck}\,\mathrm{d}k, \tag{2.12}$$

where we replaced the free electron $|\boldsymbol{p}|^2$ with its expectation value in Coulomb eigenstates.

Now, this expression can be integrated to give (dropping the superscript "ren" again) the following expression after using some well-known sum rule identities:

$$\Delta E_n = \frac{2\hbar e^2}{3\pi m^2 c^3}\sum_m |\langle\psi_n, \nabla\psi_m\rangle|^2\,(E_m - E_n)\ln\frac{\Lambda}{|E_m - E_n|},$$

where the ψ_n are Coulomb eigenfunctions (here of the Schrödinger operator and n is a collection of quantum numbers, so $n = 2s$ or $n = 2p$ would be possible choices), E_n their respective energies and Λ a UV cutoff which Bethe put to mc^2. After some approximations of the logarithm, and using that the sum over the matrix elements of ∇ leads to a delta function by the identity

$$\sum_n |\langle\psi_m, \nabla\psi_n\rangle|^2\,(E_n - E_m) = 2\pi e^2\int_{\mathbb{R}} |\psi_m|^2(x)\,\delta(x)\,\mathrm{d}x,$$

where the delta function comes from $\Delta V(\boldsymbol{x}) = \Delta\left(-e^2/|\boldsymbol{x}|\right) = 4\pi e^2\delta^{(3)}(\boldsymbol{x})$, Bethe found an energy shift between the $2s$ and $2p$ states of Hydrogen (the latter giving no contribution due to the delta function in the identity):

$$\Delta E_{2s-2p} \approx 1040\,\mathrm{MHz}$$

which is extremely close to the experimental value of 1057 MHz.

So, we have the

2.2.3. Essentials of Bethe's Treatment.

- Using time-dependent perturbation theory (which in itself could need a more rigorous justification), the dipole approximation (likewise, however, see [**DGK13**]), and renormalization (see above), Bethe found a logarithmically divergent expression for an energy shift.
- A cutoff at mc^2 and some more approximations of a very large logarithm lead to an impressive numerical result for the Lamb shift.
- In a relativistic treatment, *e.g.* the one presented by Bethe's PhD-student Dyson in [**Dys11**], after renormalization no cut-off is necessary and it improves the numerical predictions even further.
- Calculational observation: the appearance of a delta function in the shift leaves states with non-vanishing angular momentum unaltered.
- The suggested physical origin is somehow hidden in the renormalization, but could be stated as: *A back-reaction of the photonic vacuum on charged particles, which differs between bound and free states, leads to a mass or equivalently energy difference between different Hydrogen states.*

2.3. Welton's Treatment of the Lamb Shift

In his paper "Some Observable Effects of the Quantum-Mechanical Fluctuations of the Electromagnetic Field" [**Wel48**], Welton provided what the previous treatment by Bethe hardly mentioned and what disappeared again in the formalized framework of QED: an intuitive picture for the origin of the Lamb shift.

Starting from the assumption that the electromagnetic field, even in its vacuum state, fluctuates on the quantum mechanical level, he showed that such a fluctuation leads to fluctuations in the motion of charged particles[2] which in turn change the potential a bound electron "feels". The expectation of this shifted potential energy is then claimed to be the Lamb shift, and a quick calculation (it is even the one to be found on the wikipedia page of the Lamb shift) then reproduces exactly Bethe's nonrelativistic result.

2.3.1. Essentials of Welton's Treatment.

- It is the first (and to our knowledge only) approach that is both clear in physical reasoning and gives correct results (apart from questions of UV divergence and so on, see below).

[2]One might think that these are connected to the infamous zitterbewegung of Dirac's theory, but this is at least not completely true as even uncharged particles perform such a zitterbewegung – and it might also only be a sign that it is not a good idea to use the position operator to talk about (especially free!) motion of particles. We know from quantum vs. Bohmian mechanics that "true" (at least according to the theory) position and measured position (described by the operator) need not align.

- There are some finer questions as to why these fluctuations only shift the potential energy and do not increase the kinetic energy.
- Taking the fluctuations of the field seriously would again lead to infinite results as oscillations in position due to interaction with the electromagnetic field are of course divergent if the fluctuations of the field become infinite. Maybe a better relativistic approach could mend this, similar to the no longer diverging expression in the relativistic treatment of Bethe's ansatz.
- In short, the physical origin of the Lamb shift is argued to be *oscillations in the motion of an electron caused by fluctuations in the photonic field which in turn change how strongly the Coulomb potential of the nucleus acts on the electron.*

2.4. Summary

The Lamb shift, the celebrated beginning of the success of modern quantum field theory, is remarkably badly understood. There is no approach to it which does not involve divergent mathematics, and most do not even give a clear physical picture. All mentioned derivations have one idea in common, though: that somehow there is either a back-reaction of the photon field onto the electron or a pure self-interaction of the electron at heart of the Lamb shift.

We know from Dirac's treatment in [**Dir38**] that self-interaction is produced by "one-half retarded minus one-half advanced potential" of an accelerated charge. On the other hand, this just gives rise to radiation effects. It is therefore not unreasonable to suspect that the Lamb shift is related to radiative processes. We shall try to see if this is in fact correct.

CHAPTER 3

Radiation Reaction as a Toy Model

What we have seen so far hints at radiation reaction being the source of the Lamb shift. This suggests studying implementations of radiation-like quantities into quantum mechanics. Since radiation reaction effectively only depends on the motion of the test charge itself, we would like to avoid a heat-bath scenario and focus on effective one-particle descriptions instead. Two possibilities come to mind:

- Try to extend the usual quantum mechanical formalism in such a way that dissipative effects ($\propto \dddot{\boldsymbol{x}}$) can be included and give the right equations of motion, or
- to construct an effective perturbation to the Hamiltonian which might not lead to the correct equations of motion but which incorporates the main features of radiation reaction.

The first approach would obviously be preferable, but a consistent Hamiltonian or Lagrangian description for dissipative processes is not known, not even classically, apart from using dissipation functions. We develop a classical formalism, which might give rise to a quantum mechanical one similarly to the Schrödinger description being developed analogously to Hamilton-Jacobi theory, but this problem seems difficult and literature is sparse owing to the success of using open quantum systems to adress questions of dissipative nature. Another realisation of this first idea was suggested by Bennett [**Ben87**], which applies to both classical and quantum mechanics. We shall investigate this approach and find that it provides good insight into what objects to consider for our question at hand, which we then pursue as inspiration for the second idea: we compute $\dddot{\boldsymbol{x}}$ using the Heisenberg equation of motion for time-dependent operators and study several ways to construct perturbations to the Hamiltonian of the Coulomb problem. On this level, difficulties arising due to either the appearance of δ-distributions or the loss of linearity of the Hamiltonian are not severe.

3.1. Dissipative Classical Mechanics: Fractional Derivatives and the Riemann-Liouville Integral

The usual way to deal with dissipation in, say, Lagrangian mechanics is to include a dissipation function, in a sense as a generalised force, see [**LL87**]. It would be preferable,

however, to describe the entire dynamics in the Lagrangian, especially since we then might hope for a straight-forward way to study a quantum-mechanical version of the original classical system. The same idea holds true for Hamiltonian mechanics as well. However, since quantum-mechanical friction effects are usually negligible and find full treatment in the theory of open quantum systems, dissipation has not been widely adressed on the level of Lagrangians or Hamiltonians in quantum mechanics, and also in classical mechanics, there are few approaches to be found.

3.1.1. Fractional Derivatives. The usual friction term is proportional to the velocity of a particle $\dot{\boldsymbol{x}}$. Given the structure of Euler-Lagrange equations, there is no reasonable way of including a term to the Lagrange function which would yield a $\dot{\boldsymbol{x}}$-dependence after computing the Euler-Lagrange equations. A possibe way out could be found in the rarely adopted fractional calculus, as defined by the Riemann-Liouville integral, see [**Rie96**], [**Rie97**], [**Agr02**], [**Kob40**]. Especially, there is an integration by (fractional) parts for the Riemann-Liouville fractional integral [**LY38**]. The road towards a fractional calculus seems straight-forward at first, noting that the differentiation rule for monomials (and thus polynomials and even rational functions other than the pathological $1/x$) generalises easily to real-valued derivatives by using the gamma function:

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}x^k = \frac{k!}{(n-k)!}x^{k-n}$$

for integers $n \geq 0$ and $k \neq -1$ generalises to

$$\frac{\mathrm{d}^\alpha}{\mathrm{d}x^\alpha}x^r = \frac{\Gamma(r+1)}{\Gamma(\alpha-r+1)}x^{r-\alpha},$$

for $\alpha \in \mathbb{R}^+$ and $r \in \mathbb{R} \setminus \{-1\}$.

However, this is not a good definition, as it does not extend to the exponential function, even though the latter is given by a convergent power series. A better construction of a fractional derivative is the following, where first a fractional integral is introduced and then differentiated an integer amount of times:

Definition. *The* fractional derivative *of order $\alpha \in \mathbb{R}^+$ with anchor point $a \in \mathbb{R}$ of a function $f : \mathbb{R} \to \mathbb{R}$ is given by*

$$\frac{\mathrm{d}^\alpha}{\mathrm{d}(x-a)^\alpha}f(x) = \frac{\mathrm{d}^n}{\mathrm{d}x^n}\frac{1}{\Gamma(\nu)}\int_a^x \frac{f(t)}{(t-x)^{1-\nu}}\,\mathrm{d}t$$

where $n = \min\{s \in \mathbb{N} : s > \alpha\}$ *and* $\nu = n - \alpha$*, with obvious extensions to higher dimensions*[1]*. Negative order differentials are given by the* fractional integral*, so for* $\beta \in \mathbb{R}^-$*:*

$$\frac{\mathrm{d}^\beta}{\mathrm{d}(x-a)^\beta} f(x) = \frac{1}{\Gamma(-\beta)} \int_a^x \frac{f(t)}{(t-x)^{1-\beta}}\,\mathrm{d}t.$$

It is noteworthy that this notion of a fractional derivative intertwines the local aspects of the differential with the global behaviour of the function via the integral – in a sense, this matches our intuition of friction terms which as a force depend on the current velocity (or the third time derivative of the position in case of radiation reaction) but as an energy on the whole trajectory. The following theorem, which we quote without proof, shows that this mixing of differentiation and integration even extends to an integration by parts:

THEOREM 3.1 ([**LY38**]). *The fractional derivative permits an integration by parts of the following form for functions* f *and* g *mapping* $\mathbb{R} \to \mathbb{R}$ *and* $\alpha \in \mathbb{R}^+$*:*

$$\int_a^b \left(\frac{\mathrm{d}^\alpha}{\mathrm{d}(x-a)^\alpha} f(x)\right) g(x)\,\mathrm{d}x = (-1)^{-\alpha} \int_a^b f(x) \left(\frac{\mathrm{d}^\alpha}{\mathrm{d}(x-b)^\alpha} g(x)\right)\,\mathrm{d}x,$$

provided the boundary terms vanish, which we shall assume.

3.1.2. Towards a Lagrangian Formalism Including Fractional Derivatives. Using these notions, we can add a term to the Lagrangian which will produce a friction term of the desired form in the Euler-Lagrange equations, where we make use of the fractional derivative in the time coordinate.

To this end, we need to perform a variation of a Lagrange function $L = L\big(x, \dot{x}, \frac{\mathrm{d}^\alpha x}{\mathrm{d}t^\alpha}\big)$. The reasoning is simply the same as for ordinary Lagrange functions: L is a functional of the independent functions $x, \dot{x}, \frac{\mathrm{d}^\alpha x}{\mathrm{d}t^\alpha}$, which are varied. Then integration by parts allows us to use the fundamental lemma of the calculus of variations:

LEMMA (Fundamental lemma of the calculus of variations). *A continuous function* f *on an open interval* (a, b) *vanishes on that interval if for all smooth and compactly supported functions* φ *on the interval the following holds:*

$$\int_a^b f(x)\,\varphi(x)\,\mathrm{d}x = 0,$$

with which, following the standard procedure, we can derive Euler-Lagrange equations of motion for a Lagrange function involving fractional derivatives, see *e.g.* [**Rie96**].

[1] Compare with [**Rie96**].

3.1.2.1. *Example: Freely Moving Particle With Drag*[2]. For a particle with mass m moving in one dimension and experiencing drag which we want to describe for times $t \in [a, b]$, we posit the following Lagrangian:

$$L = \frac{m}{2}\dot{x}^2 + \frac{\gamma}{2}\left(\frac{\mathrm{d}^{1/2}}{\mathrm{d}(t-a)^{1/2}}x\right)^2.$$

Now, let us introduce new coordinates: $q_{1/2} := \mathrm{d}^{1/2}/\mathrm{d}(t-a)^{1/2}x, q_1 := \dot{x}$, with which we get

$$L = \frac{\gamma}{2}q_{1/2}^2 + \frac{m}{2}q_1^2.$$

The Euler-Lagrange equation of motion is then

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial q_1} &= (-1)^{-1/2}\frac{\mathrm{d}^{1/2}}{\mathrm{d}(t-b)^{1/2}}\frac{\partial L}{\partial q_{1/2}} \\ m\ddot{x} &= -\mathrm{i}\gamma\frac{\mathrm{d}^{1/2}}{\mathrm{d}(t-b)^{1/2}}\frac{\mathrm{d}^{1/2}}{\mathrm{d}(t-a)^{1/2}}x.\end{aligned}$$

Now, to arrive at the well-known actual equation of motion with linear drag $m\ddot{x} = -\beta\dot{x}$, we have to let a tend to b from below which completely negates all of the ideas behind the principle of least action[3]. Taking it as a formal trick works, but going any further with this seems a waste of time, so we will not follow this approach any further. It should be mentioned, however, that in [**Rie97**] a quantum mechanical version of this is discussed, but we will not go into this.

[2]This is a strange way to denote things. We mean: no potential, just damping proportional to the particle's velocity.

[3]Not to mention questions like "are the fractional derivatives velocity-like or coordinate-like in the Lagrangian? What physically do they mean? What about Noether's theorem (well, in fact, including friction and demanding conserved quantities is maybe not feasible – but still, what about all the elegant ways to extract information about the system just from its Lagrangian)?

3.2. Bennett's Approach

Another way to try to include radiative effects in a Lagrangian was introduced by Bennett in [**Ben87**], already in view of electromagnetic radiation and its $\dddot{x}$-term. We shall quickly introduce the idea but with a linear drag instead.

The key idea is that effective terms like the $\dot{x}$ of linear friction are not actually dynamic but effective stand-ins for the complicated processes when a particle interacts dissipatively with its environment. To remind us of this, we shall underline terms of only effective nature. Thus, in a Lagrangian like

$$L = \frac{m}{2}\dot{x}^2 - \gamma x \underline{\dot{x}} - V(x)$$

we do not vary with respect to the underlined effective quantity. The Euler-Lagrange equations of motion would yield

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} &= \frac{\partial L}{\partial x} \\ m\ddot{x} &= -\gamma \underline{\dot{x}} - \frac{\partial V(x)}{\partial x} \end{aligned}$$

thus arriving at the correct expression for linear drag. Passing to quantum mechanics via a path integral or straight-forwardly "quantising" the Hamiltonian function immediately derived from such a Lagrangian leads to a Schrödinger-like equation of the form

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\Delta\psi + \gamma x \underline{\dot{x}}\psi + V(x)\,\psi.$$

Since the effective underlined quantity is due to interaction with the environment, it is especially a classical quantity and can thus be replaced by its expectation value, so $\underline{\dot{x}} = \langle\dot{x}\rangle$, where we implicitly construct a state-dependent quantity and the inclusion of $\langle\dot{x}\rangle$ into the Hamiltonian would leave us with a non-linear operator. Apart from that, the equation for the expectation of the position operator then corresponds exactly to the classical equation:

$$m\langle\ddot{x}\rangle = -\gamma\langle\dot{x}\rangle - \langle\frac{\partial V(x)}{\partial x}\rangle.$$

3.2.1. Including Radiation Reaction. Since in the case of radiation friction, the dissipative term has the form $+(2/3)\,(e^2/c^3)\,\dddot{x}$, we postulate a Lagrangian as follows:

$$L = \frac{m}{2}\dot{x}^2 + \frac{2}{3}\frac{e^2}{c^3}\underline{\ddot{x}}x - V(x)\,,$$

which yields a quantum-mechanical Hamiltonian

$$H = -\frac{\hbar^2}{2m}\Delta + V(x) - \frac{2}{3}\frac{e^2}{c^3}\langle\ddot{x}\rangle x,$$

which, again, is in fact state-dependent and whose expectation differs from that of a non-radiating Hamiltonian with the same potential H_0 as

$$\langle H - H_0 \rangle = -\frac{2}{3}\frac{e^2}{c^3}\langle \dddot{x} \rangle \langle x \rangle. \tag{3.1}$$

Even though the derivation seems a bit like cheating, we shall in the following consider expressions similar to the one we just derived.

3.3. An Operator Ansatz

Inspired by the approaches above, we now consider a perturbation to the Hamiltonian of the form $\dddot{\boldsymbol{x}} \cdot \boldsymbol{x}$, in two different manifestations. First, let us look at the following term:

$$W := -\frac{2}{3}\frac{e^2}{c^3}\dddot{\boldsymbol{x}} \cdot \boldsymbol{x}, \tag{3.2}$$

where $\dddot{\boldsymbol{x}}$ is computed using the Heisenberg equations of motion. We should remark on slightly different choices we could make here.

3.3.1. Justification of the Choice of Eq. (3.2). The general form of equation (3.2) comes from equation (3.1), but instead of taking the product of the expectations, we first compute the scalar product $\dddot{\boldsymbol{x}} \cdot \boldsymbol{x}$ and then take its expectation value. We shall remark on the original idea below, see section 3.4. In principle there is no completely convincing argument against including an arbitrary phase factor $\mathrm{e}^{\mathrm{i}\gamma}$ for some $\gamma \in [0, 2\pi)$. An imaginary prefactor will, as becomes clear after the calculation, lead to an actual energy shift, whereas the choice made in equation (3.2) gives a purely imaginary contribution and thus a decay. But since we did not find such an imaginary prefactor in equation (3.1), we stick to the definition in eq. (3.2).

3.3.2. Calculation of Eq. (3.2). Using the shorthand $x := |\boldsymbol{x}|$, we calculate $\dddot{\boldsymbol{x}} \cdot \boldsymbol{x}$ in components[4] using the Heisenberg equation of motion for $\dddot{\boldsymbol{x}}$, where we take take the Schrödinger Hamiltonian with

$$V(\boldsymbol{x}) = -Ze^2/|\boldsymbol{x}| = -Ze^2/x :$$

[4]It is in fact quicker to calculate using coordinates since otherwise we had to use rather long expressions for vectorial Laplacians.

$$
\begin{aligned}
\dddot{x}_j x_j\varphi &= \frac{\mathrm{i}}{\hbar}\left[H,\ddot{x}_j\right]x_j\varphi \\
&= \frac{\mathrm{i}}{\hbar}\left[H,-\frac{1}{m}\partial_j V(x)\right]x_j\varphi \\
&= \frac{\mathrm{i}}{\hbar}\left[H,\frac{Ze^2}{m}\partial_j\frac{1}{x}\right]x_j\varphi \\
&= \frac{\mathrm{i}Ze^2}{\hbar m}\left[-\frac{\hbar^2}{2m}\Delta,\partial_j\frac{1}{x}\right]x_j\varphi \\
&= -\frac{\mathrm{i}Ze^2\hbar}{2m^2}\left\{\Delta\left(\left(\partial_j\frac{1}{x}\right)x_j\varphi\right)-\left(\partial_j\frac{1}{x}\right)\Delta\left(x_j\varphi\right)\right\} \\
&= -\frac{Zi\hbar}{2}\frac{e^2}{m^2}\left\{\sum_i\partial_i\left(\left(\partial_i\partial_j\frac{1}{x}\right)x_j\varphi+\partial_j\frac{1}{x}\left(\partial_i x_j\right)\varphi+\partial_j\frac{1}{x}x_j\partial_i\varphi\right)-\right. \\
&\left.-\partial_j\frac{1}{x}\sum_i\partial_i\left(\left(\partial_i x_j\right)\varphi+x_j\partial_i\varphi\right)\right\} \\
&= -\frac{Zi\hbar}{2}\frac{e^2}{m^2}\left\{\sum_i\partial_i\left(\left(\partial_i\partial_j\frac{1}{x}\right)x_j\varphi+\partial_j\frac{1}{x}\left(\delta_{ij}\right)\varphi+\partial_j\frac{1}{x}x_j\partial_i\varphi\right)-\right. \\
&\left.-\partial_j\frac{1}{x}\sum_i\partial_i\left(\left(\delta_{ij}\right)\varphi+x_j\partial_i\varphi\right)\right\}.
\end{aligned}
$$

Performing all derivatives leads to the following lengthy expression:

$$
\begin{aligned}
&= -\frac{Zi\hbar}{2}\frac{e^2}{m^2}\sum_i\left\{\left(\left(\partial_i^2\partial_j\frac{1}{x}\right)x_j\varphi+\left(\partial_i\partial_j\frac{1}{x}\right)\delta_{ij}\varphi+\left(\partial_i\partial_j\frac{1}{x}\right)x_j\partial_i\varphi+\right.\right. \\
&+\left(\partial_j\partial_j\frac{1}{x}\right)\delta_{ij}\varphi+\left(\partial_j\frac{1}{x}\right)\left(\partial_i\delta_{ij}\right)\varphi+\left(\partial_j\frac{1}{x}\right)\delta_{ij}\partial_i\varphi+ \\
&+\left(\partial_i\partial_j\frac{1}{x}\right)x_j\partial_i\varphi+\left(\partial_j\frac{1}{x}\right)\delta_{ij}\partial_i\varphi+\left(\partial_j\frac{1}{x}\right)x_j\partial_i^2\varphi\Big)- \\
&\left.\left.-\left(\left(\partial_i\delta_{ij}\right)\left(\partial_j\frac{1}{x}\right)\varphi+2\left(\partial_i x_j\right)\left(\partial_j\frac{1}{x}\right)\partial_i\varphi+\left(\partial_j\frac{1}{x}\right)x_j\partial_i^2\varphi\right)\right\}.
\end{aligned}
$$

Taking derivatives of Kronecker deltas sets some of these terms to zero, others add up:

$$
\begin{aligned}
&= -\frac{Zi\hbar}{2}\frac{e^2}{m^2}\sum_i\left\{\left(\partial_i^2\partial_j\frac{1}{x}\right)x_j\varphi+2\left(\partial_i\partial_j\frac{1}{x}\right)\delta_{ij}\varphi+2\left(\partial_i\partial_j\frac{1}{x}\right)x_j\partial_i\varphi+2\left(\partial_j\frac{1}{x}\right)\delta_{ij}\partial_i\varphi+\right. \\
&\left.+\left(\partial_j\frac{1}{x}\right)x_j\partial_i^2\varphi-2\left(\partial_j\frac{1}{x}\right)\delta_{ij}\partial_i\varphi-\partial_j\frac{1}{x}x_j\partial_i^2\varphi\right\} \\
&= -\frac{Zi\hbar}{2}\frac{e^2}{m^2}\left\{\left(\Delta\partial_j\frac{1}{x}\right)x_j\varphi+2\left(\partial_j^2\frac{1}{x}\right)\varphi+2\sum_i\left(\partial_i\partial_j\frac{1}{x}\right)x_j\partial_i\varphi\right\}.
\end{aligned}
$$

In the first term, we exchange the order of differentiation, which is allowed for all test functions φ if we understand $1/x$ as a distribution and all derivatives acting on it as distributional ones.

$$= -\frac{Z\mathrm{i}\hbar}{2}\frac{e^2}{m^2}\left\{\partial_j\left(-4\pi\delta^3(x)\right)x_j\varphi + 2\left(\partial_j^2\frac{1}{x}\right)\varphi + 2\sum_i\left(\partial_i\partial_j\frac{1}{x}\right)x_j\partial_i\varphi\right\}$$

Now we perform the summation over j as well:

$$\begin{aligned}\dddot{\boldsymbol{x}}\cdot\boldsymbol{x}\varphi &= \sum_j \dddot{x}_j x_j\varphi \\ &= -\frac{Z\mathrm{i}\hbar}{2}\frac{e^2}{m^2}\left\{-4\pi\left(\nabla\delta^3(x)\right)\cdot\boldsymbol{x}\varphi - 8\pi\delta^3(x)\,\varphi + 2\left(\left(\boldsymbol{x}\cdot\nabla\right)\nabla\frac{1}{x}\right)\cdot\nabla\varphi\right\}.\end{aligned}$$

The last term, $2\left(\left(\boldsymbol{x}\cdot\nabla\right)\nabla 1/x\right)\cdot\nabla\varphi$, is easily evaluated after going to spherical polar coordinates and gives $4/r^2\cdot\partial_r\varphi$, where r is the radial component. With this, we finally get

$$\dddot{\boldsymbol{x}}\cdot\boldsymbol{x}\varphi = -\frac{Z\mathrm{i}\hbar}{2}\frac{e^2}{m^2}\left\{-4\pi\left(\nabla\delta^3(x)\right)\cdot\boldsymbol{x}\varphi - 8\pi\delta^3(x)\,\varphi + \frac{4}{r^2}\partial_r\varphi\right\}.$$

Hence, the operator with which we perturb the Coulomb Hamiltonian reads

$$\begin{aligned}W &= -\frac{2}{3}\frac{e^2}{c^3}\dddot{\boldsymbol{x}}\cdot\boldsymbol{x} \\ &= \frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}\left\{-4\pi\left(\nabla\delta^3(x)\right)\cdot\boldsymbol{x} - 8\pi\delta^3(x) + \frac{4}{r^2}\partial_r\right\}. \qquad (3.3)\end{aligned}$$

The appearance of δ-distributions and their derivatives indicates that W is not an operator mapping $L^2\left(\mathbb{R}^3\right) \to L^2\left(\mathbb{R}^3\right)$ but rather a form on a subset[5]. However, this poses no problem due to the following reasoning:

- In conventional treatments of the Lamb shift, both the energy shift and the line width appear at first order perturbation theory, in QED this is referred to as "first loop order".
- The lowest order of perturbation theory which gives any result in our treatment should thus be the highest order to consider. As it turns out, first order perturbation theory will be sufficient.
- To first order in perturbation theory, we only compute expectation values of W in Hydrogen states. These calculations are fully well-defined.

[5]We are going to use C_c^∞ in what follows later. Of course, the standard density arguments expand all results and we can use the Hydrogen eigenfunctions, which are smooth everywhere away from zero, continuous everywhere and have a limit for the first derivative approaching zero.

Given this, we can calculate $\langle\varphi, W\psi\rangle$ for $\varphi, \psi \in C_c^\infty\big(\mathbb{R}^3\big)$ as follows, using that for a distribution $u \in \mathcal{D}'\big(\mathbb{R}^3\big)$ (the space of distributions on $C_c^\infty\big(\mathbb{R}^3\big)$) and a test function $\varphi \in C_c^\infty\big(\mathbb{R}^3\big)$, the distributional derivative $\partial_i u$, for $i = 1, 2, 3$ is again a distribution, defined by

$$\int_{\mathbb{R}^3} (\partial_i u)\, \varphi \, \mathrm{d}^3x = -\int_{\mathbb{R}^3} u \partial_i \varphi \, \mathrm{d}^3x :$$

$$\begin{aligned}\langle\varphi, W\psi\rangle &= \frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}\langle\varphi, \left(-4\pi\left(\nabla\delta^3(x)\right)\cdot\boldsymbol{x} - 8\pi\delta^3(x) + \frac{4}{r^2}\partial_r\right)\psi\rangle \\ &= \frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}\int \varphi^*(x)\left(\underbrace{-4\pi\left(\nabla\delta^3(x)\right)\cdot\boldsymbol{x}}_{(*)} - 8\pi\delta^3(x) + \frac{4}{r^2}\partial_r\right)\psi(x)\ \mathrm{d}^3x.\end{aligned}$$

Evaluating the $(*)$-part of the parentheses without the constants in front of the integral gives:

$$\begin{aligned}\frac{1}{-\frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}}(*) &= 4\pi\int \delta^3(x)\,\nabla\cdot\left(\varphi^*(x)\,\psi(x)\,\boldsymbol{x}\right)\,\mathrm{d}^3x \\ &= 4\pi\int \delta^3(x)\left(3\varphi^*(x)\,\psi(x) + \boldsymbol{x}\cdot\nabla\left(\varphi^*(x)\,\psi(x)\right)\right)\,\mathrm{d}^3x \\ &= 12\pi\int \delta^3(x)\,\varphi^*(x)\,\psi(x)\,\mathrm{d}^3x,\end{aligned}$$

where we integrated by parts in the first line. With this we find

$$\langle\varphi, W\psi\rangle = \frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}\int \varphi^*(x)\left(4\pi\delta^3(x) + \frac{4}{r^2}\partial_r\right)\psi(x)\ \mathrm{d}^3x. \tag{3.4}$$

We thus are to compute the expectation values of W in the $2s$ and the $2p$ states of the Hydrogen atom. The respective wave functions in spherical polar coordinates are given as:

$$\psi_{2s}(r,\theta,\varphi) = \left(\frac{Z}{a_0}\right)^{3/2}\frac{1}{\sqrt{8\pi}}\left(1 - \frac{Z}{2a_0}r\right)\mathrm{e}^{-\frac{Z}{2a_0}r}, \tag{3.5}$$

$$\psi^0_{2p}(r,\theta,\varphi) = \left(\frac{Z}{a_0}\right)^{5/2}\frac{1}{\sqrt{32\pi}}r\cos\theta\mathrm{e}^{-\frac{Z}{2a_o}r}, \tag{3.6}$$

$$\psi^\pm_{2p}(r,\theta,\varphi) = \mp\left(\frac{Z}{a_0}\right)^{5/2}\frac{1}{\sqrt{8\pi}}r\sin\theta\mathrm{e}^{-\frac{Z}{2a_0}r}\mathrm{e}^{\pm\mathrm{i}\varphi}. \tag{3.7}$$

Let us first consider the expectation value of W in any of the three $2p$-states. It is clear that the contribution of the $\delta^3(x)$-term in equation (3.4) is zero for all p-states since parity requires them to vanish at the origin. This means that the only nonvanishing term

can come from the radial derivative. Ignoring the straightforward θ- and φ-dependencies of equations (3.6) and (3.7), the radial integrals we have to perform after taking the derivative are of the form

$$\int_0^\infty r\left(1-\frac{Z}{2a_0}r\right)\mathrm{e}^{-\frac{Z}{a_0}r}\,\mathrm{d}r=0,$$

which is easily calculated after substituting $r\to R:=\frac{Z}{a_0}r$.

Thus, $\langle\psi_{2p},W\psi_{2p}\rangle=0$ for all three $2p$-states, and it remains to compute $\langle\psi_{2s},W\psi_{2s}\rangle$. To this end, we first take the radial derivative of $\psi_{2s}(x)$:

$$\partial_r\psi_{2s}(r,\theta,\varphi)=-\frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{5/2}\left(2-\frac{Z}{2a_0}r\right)\mathrm{e}^{-\frac{Z}{2a_0}r}.$$

Now it is a straightforward calculation to find the expectation of W in the $2s$-state:

$$\begin{aligned}\langle\psi_{2s},W\psi_{2s}\rangle&=\frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}\Bigg(4\pi\left|\psi_{2s}(0)\right|^2-\\&\quad-4\int_0^{2\pi}\mathrm{d}\varphi\int_{-1}^{1}\mathrm{d}u\int_0^\infty\mathrm{d}r\,r^2\left(\frac{Z}{a_0}\right)^4\frac{1}{16\pi}\left(1-\frac{Z}{2a_0}r\right)\frac{1}{r^2}\left(2-\frac{Z}{2a_0}r\right)\mathrm{e}^{-\frac{Z}{a_0}r}\Bigg)\\&=\frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}\left(4\pi\left|\psi_{2s}(0)\right|^2-\left(\frac{Z}{a_0}\right)^4\int_0^\infty\mathrm{d}r\,\left(1-\frac{Z}{2a_0}r\right)\left(2-\frac{Z}{2a_0}r\right)\mathrm{e}^{-\frac{Z}{a_0}r}\right),\end{aligned}$$

which we compute by substituting $r\to R:=\frac{Z}{a_0}r$:

$$\begin{aligned}&=\frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}\left(4\pi\left|\psi_{2s}(0)\right|^2-\left(\frac{Z}{a_0}\right)^3\underbrace{\int_0^\infty\mathrm{d}R\,\left(1-\frac{R}{2}\right)\left(2-\frac{R}{2}\right)\mathrm{e}^{-R}}_{=1}\right)\\&=\frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}\left(4\pi\left|\psi_{2s}(0)\right|^2-\left(\frac{Z}{a_0}\right)^3\right).\end{aligned}$$

The value at the origin is well-known for all Coulomb wave functions, and found to be $|\psi_{2s}(0)|^2=1/(8\pi)\,(Z/a_0)^3$,

$$\begin{aligned}&=\frac{Z\mathrm{i}\hbar}{3}\frac{e^4}{m^2c^3}\left(\frac{1}{2}\left(\frac{Z}{a_0}\right)^3-\left(\frac{Z}{a_0}\right)^3\right)\\&=-\frac{Z\mathrm{i}\hbar}{6}\frac{e^4}{m^2c^3}\left(\frac{Z}{a_0}\right)^3.\end{aligned}$$

If we express the Bohr radius in terms of atomic constants, it reads $a_0 = \hbar^2/(me^2)$, thus we finally arrive at

$$\begin{aligned}\langle \psi_{2s}, W\psi_{2s}\rangle &= -\frac{\mathrm{i}}{6} Z^4 \frac{me^1 0}{c^3\hbar^5} \\ &= -\frac{\mathrm{i}}{6} Z^4 mc^2\alpha^5, \end{aligned} \tag{3.8}$$

with $\alpha = e^2/(\hbar c) \approx 1/137$ being the fine-structure constant.

3.3.3. Discussion of the Result in Eq. (3.8). Even before computing the numerical value of equation (3.8), we observe several facts:

- The result behaves like α^5, which is the same dependence on α as in QED calculations of the Lamb shift, see example [**Wei05**]. However, the numerical factors differ.
- More importantly, we obtain an entirely imaginary perturbation, which is somewhat surprising and needs explanation.

Following the example by Gamow in [**Gam28**] and the treatment in [**LL92**], we recognize that complex energies produce two effects: Their real parts correspond to an energy shift (which is completely absent here) while the imaginary part produces a decay: Splitting a complex energy E into its real and imaginary parts as $E = \Delta E - \mathrm{i}\frac{\Gamma}{2}$ leads to an exponentially decaying (generalised eigen-)state ψ:

$$\begin{aligned}|\psi_t|^2 &= \left|\mathrm{e}^{-\mathrm{i}tE/\hbar}\psi_0\right|^2 \\ &= \left|\mathrm{e}^{-\mathrm{i}t\Delta E/\hbar}\mathrm{e}^{-\Gamma/(2\hbar)t}\psi_0\right|^2 \\ &= |\psi_0|^2\,\mathrm{e}^{-\Gamma/\hbar\cdot t}. \end{aligned}$$

This indicates that the lifetime of a state with decay constant Γ is $\tau = \hbar/\Gamma$.

With this in mind, we find that $\Gamma_{2s} = \frac{Z^4}{3} mc^2\alpha^5$ and thus

$$\tau_{2s} = \frac{3\hbar}{Z^4 mc^2\alpha^5},$$

which in Hydrogen ($Z = 1$) yields

$$\tau_{2s} = 1.877 \cdot 10^{-10} s. \tag{3.9}$$

Given that the $2s$ state is known to be quite long lived (due to selection rules the decay $2s \to 1s$ is only possible via a two-photon process and thus suppressed), this number really does not match our expectations. But it is only about a factor 10 away from the lifetime of the $2p$ state, which is found as $1.596 \cdot 10^{-9} s$ [**WF09**].

Granted, these are not remarkably close numbers, especially since the behaviour of the lifetimes does not respect the selection rules.

But this toy model still shows two things:

- A radiation reaction, even if implemented only in an *ad-hoc* manner, yields a correspondingly crude estimate of a central QED-like effect, that is, the line-width part of the Lamb shift.
- However, no energy shift is found, and the behaviour seems not to respect selection rules.

Before we continue with a totally different approach, let us quickly revisit the original expression we found in equation (3.1).

3.4. Another Implementation

Instead of equation (3.2), and now closer to what we found in equation (3.1), we can consider a different construction of a radiative contribution to the Hamiltonian: For a state ψ define

$$U_\psi := -\frac{2}{3}\frac{e^2}{c^3}\langle\psi, \dddot{\boldsymbol{x}}\psi\rangle \cdot \boldsymbol{x}. \tag{3.10}$$

In order to put this expression to use, we need to compute $\dddot{\boldsymbol{x}}\varphi$ for $\varphi \in C_c^\infty$:

$$\begin{aligned}
\dddot{\boldsymbol{x}}\varphi &= \frac{\mathrm{i}}{\hbar}\left[H, \ddot{\boldsymbol{x}}\right]\varphi \\
&= \frac{\mathrm{i}}{\hbar}\left[H, -\frac{1}{m}\nabla V(x)\right]\varphi \\
&= \frac{\mathrm{i}}{\hbar}\left[-\frac{\hbar^2}{2m}\Delta, -\frac{1}{m}\nabla V(x)\right]\varphi \\
&= \frac{\mathrm{i}\hbar}{2m^2}\left\{\Delta\nabla V(x) - \nabla V(x)\,\Delta\right\}\varphi \\
&= \frac{\mathrm{i}\hbar}{2m^2}\left\{(\Delta\nabla V(x)) + 2\,(\Delta V(x))\,\nabla\right\}\varphi.
\end{aligned}$$

Evaluating this as quadratic form gives

$$\begin{aligned}
\langle\varphi, \dddot{\boldsymbol{x}}\varphi\rangle &= \frac{\mathrm{i}\hbar}{2m^2}\langle\varphi, \left\{(\Delta\nabla V(x)) + 2\,(\Delta V(x))\,\nabla\right\}\varphi\rangle \\
&= \frac{\mathrm{i}\hbar}{2m^2}\left\{\langle\varphi, (\Delta\nabla V(x))\,\varphi\rangle + 2\langle\varphi, (\Delta V(x))\,\nabla\varphi\rangle\right\} \\
&= \frac{\mathrm{i}\hbar}{2m^2}\left\{\int \varphi^*(x)\,(\Delta\nabla V(x))\,\varphi(x)\ \mathrm{d}^3x + 2\int \varphi^*(x)\,(\Delta V(x))\,\nabla\varphi(x)\ \mathrm{d}^3x\right\} \\
&= \frac{\mathrm{i}\hbar}{2m^2}\left\{-\int (\Delta V(x))\,\nabla\left(\varphi^*(x)\,\varphi(x)\right)\ \mathrm{d}^3x + 2\int \varphi^*(x)\,(\Delta V(x))\,\nabla\varphi(x)\ \mathrm{d}^3x\right\} \\
&= \frac{\mathrm{i}\hbar}{2m^2}\left\{\int \varphi^*(x)\,(\Delta V(x))\,\nabla\varphi(x) - (\nabla\varphi^*(x))\,(\Delta V(x))\,\varphi(x)\ \mathrm{d}^3x\right\} \\
&= \frac{\mathrm{i}\hbar}{2m^2}\int (\Delta V(x))\left\{\varphi^*(x)\,\nabla\varphi(x) - \nabla\varphi^*(x)\,\varphi(x)\right\}\ \mathrm{d}^3x \\
&= \frac{\mathrm{i}\hbar}{2m^2}\int (\Delta V(x))\,2\frac{\mathrm{i}m}{\hbar}\boldsymbol{j}^\varphi(x)\ \mathrm{d}^3x \\
&= -\frac{1}{m}\int \boldsymbol{j}^\varphi(x)\,\Delta V(x)\ \mathrm{d}^3x.
\end{aligned}$$

For a point charge at the origin, this simplifies to the current at the origin which is, however, not well-defined for the Coulomb problem. If instead we take a finite and homogeneously charged ball of radius R as source of V, i.e. $\Delta V(x) = -e\rho(x)$, where

$\rho(x) = \frac{3e}{4\pi R^3} \mathbb{1}_{B_R(0)}(x)$, we find:

$$\langle \varphi, \ddot{\boldsymbol{x}} \varphi \rangle = \frac{e^2}{m} \frac{3}{4\pi R^3} \int_{B_R(0)} \boldsymbol{j}^{\varphi}(x) \, \mathrm{d}^3 x$$

which makes less problems to evaluate.

Assuming that the Hydrogen states are approximately the same for a point charge and a small sphere for the nucleus, we can compute the expectation of U_ψ in those eigenstates. It is a longer but straightforward calculation to see that $\langle U_\psi \rangle_\psi$ vanishes for Hydrogen eigenstates due to orthogonality of $\boldsymbol{j}$ and $\langle \boldsymbol{x} \rangle$.

3.5. Summary and Motivation for Another Approach

We saw in the preceding calculations that the construction $W = -\frac{2}{3}\frac{e^2}{c^3} \dddot{\boldsymbol{x}} \cdot \boldsymbol{x}$ from equation (3.2) yields an imaginary perturbation to the Hydrogen Hamiltonian. It is not clear, however, how far we can trust this ansatz. Therefore, we would like to consider a very different setup and see if we can reproduce the key features of our result, which were:

- Radiation reaction only leads to the decay widths part of the Lamb shift.
- This we get without any divergences[6].

We shall now proceed to fully relativistic quantum mechanics, *i.e.* studying the Dirac equation in a not too well-known approach due to Barut.

[6]Since we were operating on a semi-classical basis here, it is not too surprising that all our calculations went through without problems after we essentially got rid of the possibly divergent electromagnetic field.

CHAPTER 4

Barut's Self-Energy Treatment of the Lamb Shift

In a series of papers ([**BK83**], [**BV85**], [**Bar88**], [**BS88**], [**BKSÜ92**], [**ABKÜ95**]), Barut *et.al.* developed a method of describing QED effects well suited for bound states[1] avoiding quantized fields. Instead, they utilized self reaction by coupling the Dirac wave function directly to its own current[2]:

$$\begin{aligned} \left(\mathrm{i}\partial\!\!\!/ - m - eA\!\!\!/_{\mathrm{Coul}}\right)\Psi &= eA\!\!\!/_{\mathrm{self}}\Psi \\ \Box A^{\mu}_{\mathrm{self}} &= 4\pi\overline{\Psi}\gamma^{\mu}\Psi. \end{aligned} \tag{4.1}$$

The solution for A^{μ} (in the Lorenz gauge $\partial_{\mu}A^{\mu}=0$) from the last line is then given by convolution of the current against the causal propagator:

$$A^{\mu}_{\mathrm{self}}(\mathsf{x}) = -e\int D(\mathsf{x}-\mathsf{y})\,\overline{\Psi}(\mathsf{y})\,\gamma^{\mu}\Psi(\mathsf{y})\;\mathrm{d}^4y,$$

where $D(\mathsf{x}) = -\lim\limits_{\varepsilon\searrow 0}\int \frac{\mathrm{e}^{-\mathrm{i}\mathsf{q}\cdot\mathsf{x}}}{(q^0+\mathrm{i}\varepsilon)^2-\boldsymbol{q}^2}\frac{\mathrm{d}^4q}{(2\pi)^4}$, the sign of the $\mathrm{i}\varepsilon$ term signifying that the contour, which for $x^0>0$ has to be closed *below* the real axis, is to be chosen such that it includes both poles at $q^0=\pm|\boldsymbol{q}|$. From now on we write $q:=|\boldsymbol{q}|\in\mathbb{R}$, not to be confused with $\mathsf{q}\in\mathbb{R}^4$. We repeat the first part of the calculation here and then proceed to include the split of the fields which was introduced by Dirac, veryfing our finding that the radiation field produces the decay part of the Lamb shift.

Plugging everything into the first line of equation (4.1) and dropping the subscript of A_{self}, we get:

$$\begin{aligned} &\left(\mathrm{i}\partial\!\!\!/ - m - eA\!\!\!/_{\mathrm{Coul}}\right)\Psi(\mathsf{x}) \\ &= e^2\int\lim_{\varepsilon\searrow 0}\int\frac{\mathrm{e}^{-\mathrm{i}\mathsf{q}\cdot(\mathsf{x}-\mathsf{y})}}{(q^0+\mathrm{i}\varepsilon)^2-q^2}\overline{\Psi}(\mathsf{y})\,\gamma^{\mu}\Psi(\mathsf{y})\;\frac{\mathrm{d}^4q}{(2\pi)^4}\mathrm{d}^4y\,\gamma_{\mu}\Psi(\mathsf{x}) \\ &= e^2\int\lim_{\varepsilon\searrow 0}\int\frac{\mathrm{e}^{-\mathrm{i}\mathsf{q}\cdot(\mathsf{x}-\mathsf{y})}}{2q}\left\{\frac{1}{q^0+\mathrm{i}\varepsilon-q}-\frac{1}{q^0+\mathrm{i}\varepsilon+q}\right\}\overline{\Psi}(\mathsf{y})\,\gamma^{\mu}\Psi(\mathsf{y})\;\frac{\mathrm{d}^4q}{(2\pi)^4}\mathrm{d}^4y\,\gamma_{\mu}\Psi(\mathsf{x}) \\ &= e^2\iint\left\{\mathsf{P.V.}\frac{1}{q^0-q}-\mathrm{i}\pi\delta\big(q^0-q\big)-\mathsf{P.V.}\frac{1}{q^0+q}+\mathrm{i}\pi\delta\big(q^0+q\big)\right\}\overline{\Psi}(\mathsf{y})\,\gamma^{\mu}\Psi(\mathsf{y})\;\frac{\mathrm{d}^4q}{(2\pi)^4}\mathrm{d}^4y\,\gamma_{\mu}\Psi(\mathsf{x})\,, \end{aligned}$$

[1] It was applied to atomic phenomena like the Lamb shift, spontaneous emission and vacuum polarization.
[2] From now on, we will use units where $\hbar=c=1$.

where the third line comes from expanding the fraction and the fourth from using the Sokhotski-Plemelj theorem[3] for the q^0-integration.

The principal value terms will lead to a Lamb shift, while the delta functions generate a decay, as we can guess already from the appearance of a factor i in front of them.

To save some writing, let us introduce the following shorthand:

$$K\big(q^0,q\big) := \mathsf{P.V.}\frac{1}{q^0-q} - \mathrm{i}\pi\delta\big(q^0-q\big) - \mathsf{P.V.}\frac{1}{q^0+q} + \mathrm{i}\pi\delta\big(q^0+q\big)\,.$$

Now we expand all wave functions according to a time-dependent perturbation similar to the one we used in section 2.2 formally as $\Psi(\mathsf{x}) = \sum_n \mathrm{e}^{-\mathrm{i}E_n x^0}\psi_n(\boldsymbol{x})$ and proceed without worrying about exchanging sums and integrals (also the expansion of the wave function might include a continuous energy spectrum, where we should integrate instead of sum, but we neglect these questions for now):

$$\sum_n \big(\mathrm{i}\gamma^0\partial_0 + \mathrm{i}\boldsymbol{\gamma}\cdot\nabla - m - e\not{A}_{\mathrm{Coul}}\big)\,\mathrm{e}^{-\mathrm{i}E_n x^0}\psi_n(\boldsymbol{x})$$
$$= \sum_{m,r,s} e^2 \iint \frac{\mathrm{e}^{-\mathrm{i}\mathsf{q}\cdot(\mathsf{x}-\mathsf{y})}}{2q} K\big(q^0,q\big)\,\mathrm{e}^{+\mathrm{i}E_m y^0}\overline{\psi}_m(\boldsymbol{y})\,\gamma^\mu \mathrm{e}^{-\mathrm{i}E_r y^0}\psi_r(\boldsymbol{y})\;\frac{\mathrm{d}^4q}{(2\pi)^4}\mathrm{d}^4y\,\gamma_\mu \mathrm{e}^{-\mathrm{i}E_s x^0}\psi_s(\boldsymbol{x})\,.$$

Seperating the exponential including q and performing the y^0-integral followed by the q^0-integral yields:

$$= \sum_{m,r,s} e^2 \iint \frac{\mathrm{e}^{+\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{y})}}{2q} K(E_r-E_m,q)\,\mathrm{e}^{-\mathrm{i}(E_r-E_m+E_s)x^0}\overline{\psi}_m(\boldsymbol{y})\,\gamma^\mu\psi_r(\boldsymbol{y})\;\frac{\mathrm{d}^3q}{(2\pi)^3}\mathrm{d}^3y\,\gamma_\mu\psi_s(\boldsymbol{x})\,.$$

When we compare the coefficients of x^0 in the exponential on the left and right hand sides, we learn that $E_r - E_m + E_s = E_n$, which can be satisfied by choosing $E_s = E_m$ and consequently $E_n = E_r$, which implies that $\psi_s = \psi_m$ and $\psi_n = \psi_r$ as well. The other choice $E_s = E_n$ leads to vacuum polarizations terms.

If we now multiply by the n-th Coulomb wave function $\overline{\psi}^C_n(\boldsymbol{x})$ from the left and set $E_n = E^C_n + \Delta E_n$ on the left hand side, we get:

$$(\psi^C_n(\boldsymbol{x}))^\dagger\psi_n(\boldsymbol{x})\,\Delta E_n$$
$$= \sum_m e^2 \iint \frac{\mathrm{e}^{+\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{y})}}{2q} K(E_r-E_m,q)\,\overline{\psi}_m(\boldsymbol{y})\,\gamma^\mu\psi_r(\boldsymbol{y})\,\overline{\psi}^C_n(\boldsymbol{x})\,\gamma_\mu\psi_s(\boldsymbol{x})\;\frac{\mathrm{d}^3q}{(2\pi)^3}\mathrm{d}^3y.$$

In the last step, we set all wave functions equal to the respective Coulomb wave functions as a first iteration of an assumed solution method in the spirit of a von-Neumann

[3] See theorem A.1 in the Appendix.

iteration, and integrate over d^3x, keep in mind that in our choice $\psi_r = \psi_n$ and $\psi_s = \psi_m$:

$$\begin{aligned}\Delta E_n &= e^2 \sum_m \int \frac{K(E_r - E_m, q)}{2q} \left(\int \overline{\psi}^C_m(\boldsymbol{y})\, \gamma^\mu \psi^C_r(\boldsymbol{y})\, \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{y}}\, \mathrm{d}^3y \right) \times \\ &\quad \times \left(\int \overline{\psi}^C_n(\boldsymbol{x})\, \gamma_\mu \psi^C_s(\boldsymbol{x})\, \mathrm{e}^{+\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}}\, \mathrm{d}^3x \right) \frac{\mathrm{d}^3q}{(2\pi)^3} \\ &=: \frac{e^2}{(2\pi)^3} \sum_m \int K(E_r - E_m, q)\, T^\mu_{mn}(\boldsymbol{q})\, T_{nm}(-\boldsymbol{q})_\mu\, \frac{\mathrm{d}^3q}{2q}.\end{aligned}$$

Writing out $K(E_r - E_m, q)$, we find two different parts to ΔE_n:

$$\Delta E^{\mathrm{LS}}_n = \frac{e^2}{(2\pi)^3} \sum_m \int \left\{ \mathsf{P.V.}\frac{1}{q^0 - q} - \mathsf{P.V.}\frac{1}{q^0 + q} \right\} T^\mu_{mn}(\boldsymbol{q})\, T_{nm}(-\boldsymbol{q})_\mu\, \frac{\mathrm{d}^3q}{2q} \tag{4.2}$$

$$\Delta E^{\mathrm{SE}}_n = -\mathrm{i}\pi \frac{e^2}{(2\pi)^3} \sum_m \int \left\{ \delta\big(q^0 - q\big) - \delta\big(q^0 + q\big) \right\} T^\mu_{mn}(\boldsymbol{q})\, T_{nm}(-\boldsymbol{q})_\mu\, \frac{\mathrm{d}^3q}{2q} \tag{4.3}$$

The first expression can be shown using Mellin transforms to give the (real) Lamb shift (in the dipole approximation, this result goes over into Bethe's), see [**BKSÜ92, BK83**] and the second one describes spontaneous emission, see [**BS88**].

4.1. Splitting the Potentials

Now, let us look at the idea of introducing the radiation field from Wheeler-Feynman electrodynamics or equivalently from Dirac's analysis in [**Dir38**] via

$$\begin{aligned}A^\mu_{\mathrm{self}}(\mathsf{x}) &= -e \int \frac{1}{2} \left(D_{\mathrm{ret}}(\mathsf{x} - \mathsf{y}) - D_{\mathrm{adv}}(\mathsf{x} - \mathsf{y}) \right) \overline{\Psi}(\mathsf{y})\, \gamma^\mu \Psi(\mathsf{y})\, \mathrm{d}^4y, \\ D_{\mathrm{ret}}(\mathsf{x}) &= -\lim_{\varepsilon \searrow 0} \int \frac{\mathrm{e}^{-\mathrm{i}\mathsf{q}\cdot\mathsf{x}}}{\big(q^0 + \mathrm{i}\varepsilon\big)^2 - \boldsymbol{q}^2} \frac{\mathrm{d}^4q}{(2\pi)^4} \\ D_{\mathrm{adv}}(\mathsf{x}) &= -\lim_{\varepsilon \searrow 0} \int \frac{\mathrm{e}^{-\mathrm{i}\mathsf{q}\cdot\mathsf{x}}}{\big(q^0 - \mathrm{i}\varepsilon\big)^2 - \boldsymbol{q}^2} \frac{\mathrm{d}^4q}{(2\pi)^4}.\end{aligned}$$

The advanced propagator is of course to be equipped by a specific contour of integration, and for $x^0 < y^0$ this contour is to be closed *above* the real axis including the two poles.

Proceeding like above gives:

$$
\begin{aligned}
&\left(\mathrm{i}\not{\partial} - m - e\not{A}_{\mathrm{Coul}}\right)\Psi(\mathsf{x}) \\
&= e^2 \int \lim_{\varepsilon \searrow 0} \int \frac{1}{2} \mathrm{e}^{-\mathrm{i}\mathsf{q}\cdot(\mathsf{x}-\mathsf{y})} \left(\frac{1}{(q^0+\mathrm{i}\varepsilon)^2 - q^2} - \frac{1}{(q^0-\mathrm{i}\varepsilon)^2 - q^2} \right) \overline{\Psi}(\mathsf{y})\, \gamma^\mu \Psi(\mathsf{y})\ \frac{\mathrm{d}^4 q}{(2\pi)^4} \mathrm{d}^4 y\, \gamma_\mu \Psi(\mathsf{x}) \\
&= e^2 \int \lim_{\varepsilon \searrow 0} \int \frac{\mathrm{e}^{-\mathrm{i}\mathsf{q}\cdot(\mathsf{x}-\mathsf{y})}}{2 \cdot 2q} \left\{ \frac{1}{q^0 + \mathrm{i}\varepsilon - q} - \frac{1}{q^0 + \mathrm{i}\varepsilon + q} - \frac{1}{q^0 - \mathrm{i}\varepsilon - q} + \frac{1}{q^0 - \mathrm{i}\varepsilon - q} \right\} \times \\
&\times\, \overline{\Psi}(\mathsf{y})\, \gamma^\mu \Psi(\mathsf{y})\ \frac{\mathrm{d}^4 q}{(2\pi)^4} \mathrm{d}^4 y\, \gamma_\mu \Psi(\mathsf{x}) \\
&= e^2 \iint \frac{\mathrm{e}^{-\mathrm{i}\mathsf{q}\cdot(\mathsf{x}-\mathsf{y})}}{2 \cdot 2q} \left\{ \mathsf{P.V.}\frac{1}{q^0 - q} - \mathrm{i}\pi\delta\big(q^0 - q\big) - \mathsf{P.V.}\frac{1}{q^0 + q} + \mathrm{i}\pi\delta\big(q^0 + q\big) - \right. \\
&\left. -\mathsf{P.V.}\frac{1}{q^0 - q} - \mathrm{i}\pi\delta\big(q^0 - q\big) + \mathsf{P.V.}\frac{1}{q^0 + q} + \mathrm{i}\pi\delta\big(q^0 + q\big) \right\} \overline{\Psi}(\mathsf{y})\, \gamma^\mu \Psi(\mathsf{y})\ \frac{\mathrm{d}^4 q}{(2\pi)^4} \mathrm{d}^4 y\, \gamma_\mu \Psi(\mathsf{x})\,,
\end{aligned}
$$

where the principal values cancel out and the delta functions add up, removing the factor $1/2$ and leaving us with the terms for spontaneous emission from equation (4.3).

We see that the natural approach to only utilize Dirac's self-field yields no energy shift, only the line width remains. This agrees with our operator ansatz using $W = \frac{2}{3}\frac{e^2}{c^3}\dddot{\boldsymbol{x}} \cdot \boldsymbol{x}$ in equation (3.2), only now the expressions predict the correct lifetimes.

On the other hand, if we consider instead of Dirac's self-field the combination

$$A^\mu_{\mathrm{mass}}(\mathsf{x}) = -e \int \frac{1}{2} \left(D_{\mathrm{ret}}(\mathsf{x}-\mathsf{y}) + D_{\mathrm{adv}}(\mathsf{x}-\mathsf{y}) \right) \overline{\Psi}(\mathsf{y})\, \gamma^\mu \Psi(\mathsf{y})\ \mathrm{d}^4 y$$

(note the plus!), we only find the terms for the real Lamb shift as in equation (4.2).

This is *exactly* analogous to Dirac's splitting in [**Dir38**]: an infinite mass term (proportional to $D_{\mathrm{ret}} + D_{\mathrm{adv}}$, or A^μ_{mass}) plus a well-defined self-interaction term (correspondingly proportional to $D_{\mathrm{ret}} - D_{\mathrm{adv}}$, that is A^μ_{self}), here they correspond to the real Lamb shift and spontaneous emission (decay width). It should also be noted again that in Wheeler's and Feynman's derivation of the radiation reaction [**WF45**], it is shown that in the vicinity of an accelerated charge the effective field is just the usual retarded field from Maxwell electrodynamics, while the particle itself produces the fully time-symmetric retarded plus advanced field and feels its own retarded minus advanced field, thus producing an effective field in its vicinity which is fully retarded.

4.2. Summary

Barut's treatment, although using a dubiously-looking equation[4], provides a very direct approach to bound-state phenomena in QED. When splitting the self-interaction

[4]In fact, it might be an effective equation for a more fundamental description. Possibly one could understand it as a bound-state limit for QED, since similar effective equations can be found when many coherent photons are present [**Pic15**].

potential into Dirac's self-field and mass-part, we see that the Lamb shift follows this split exactly. Since the mass term is still mathematically ill-defined, it would not be true to say that this clears up the mechanism behind the Lamb shift. But it seems obvious that spontaneous emission, or equivalently decay width, is completely caused by radiative effects.

CHAPTER 5

Conclusion and Outlook

5.1. Discussion of the Physical Origin of the Lamb Shift

Our treatment seems to suggest that the two parts of the Lamb shift have different origins.

Its real part is still somewhat hidden in a divergent mass term and might be caused by one (or a combination of several) of the following effects:

- The ordinary picture of the electron dragging around its Coulomb field, giving it an additional mass contribution. However, this cannot simply be represented in Wheeler-Feynman electrodynamics, since there is no Coulomb field.
- Another option might be found in the way radiation reaction is described in WFE, see [**WF45**], [**BDDH14**]. It is plausible that the effects of the absorber back on the accelerated particle are not fully recovered by the approximations made in the cited derivations, and that better estimates lead to additional effects which in turn might establish a real Lamb shift when "quantised". Maybe the absorber has to be studied again, possibly even quantum mechanical, to get a correct view of its action on an accelerated test charge.
- As a third idea, thermodynamic effects can always be a feasible source for the Lamb shift. Compared to Brownian motion, the friction part would then find a fluctuative counterpart, which in turn would yield a behaviour similar to a fluctuation-dissipation theorem, [**CL83**]. But what would constitute the heat bath? Here anything from cosmic background radiation to the Dirac sea seems somehow imaginable, but equally unpleasant since then the Lamb shift could be used as a thermometer of the Dirac sea (or the universe as a hole, if we think of background radiation).
- Another possibility would be that the real Lamb shift originates from a true quantum mechanical effect for the electron, similar to the processes happening in Gamow decay [**DGK11**] or quite generally the theory of resonances [**BBP13**].
- Also, Welton's treatment [**Wel48**] suggests that the free part of the Dirac Hamiltonian might be responsible for the Lamb shift due to an effect similar to zitterbewegung. This seems to be the most promising idea at this point.

Of course, Wheeler-Feynman electrodynamics is far from being completely understood, and a quantum-mechanical version is not yet at hand. Still, it seems at least promising to be studied in more detail – even if a quantum formulation turns out to be impossible, the philosophical underpinnings (full time symmetry, no fields) should be understood as invitations to rethink fundamental ideas when all present theories fail to give the answers we expect from physics.

The imaginary part of the Lamb shift, connected to lifetimes of states, appears to be produced by self interaction of the electron, which would usually be referred to as radiative decay. It was claimed by some authors, *e.g.* [**DDRCT82**], that radiation alone could not be responsible for the Lamb shift. Now we see that this holds true and can even pinpoint exactly which parts of the Lamb shift are given by which phenomenon.

5.2. What Needs to be Done?

Even though some improvement in the understanding of the Lamb shift has been made, open questions remain.

5.2.1. What is the Exact Source of the Real Lamb Shift? As remarked above, this is not satisfactorially answered by our treatment, we only isolated the cause but could not give a physical answer. Following Welton, it might just make a difference if a charged particle moves freely or in a bound state or is accelerated. What about a particle moving on a Kepler orbit? Do we find a Lamb shift there as well?

5.2.2. Why This Equation? Barut's ansatz in equation (4.1) seems ad-hoc. How can it be motivated? Is it an effective equation and thus "correct" in a limiting sense? Or is it just a good guess? Or is it fundamental?[1] Going further, is it well-defined? In order to answer this, one would have to study Maxwell-Dirac systems and check their predictions, maybe using an improved version of time-dependent perturbation theory. Are there generalisations of this equation, maybe for free particles, or for many?

5.2.3. Some Speculation. Studying integral equations similar to the Bethe-Salpeter equation might give clues to a fully relativistic interacting quantum theory of light and matter. Lately, there has been some progress in this direction, see *e.g.* [**Lie15**] or [**TT15**], but so far only toy models could be handled. While not being fundamental, it might then still be useful to study equations like Barut's to get an understandig of how relativistic quantum theories produce certain phenomena.

On the other hand, directly "quantising" Wheeler-Feynman electrodynamics needs to handle this theory's delay character, which again is included in Barut's ansatz if we take the self-field to be a combination of advanced and retarded potentials. Solution

[1] This last one is probably a simple "no".

theories for extremely narrow conditions exist, see [**FST87**], but have yet to be found for a full Maxwell-Dirac system.

APPENDIX A

The Sokhotski-Plemelj Theorem

When dealing with propagators, quite often we have to integrate in the complex plane. The following theorem, which follows easily from Cauchy's integral formula, helps in these calculations.

THEOREM A.1 (Sokhotski-Plemelj). *For a function $f : \mathbb{R} \to \mathbb{C}$ which is continuous along $\mathbb{R}$ and $a, b \in \mathbb{R}$ with $a < b$, it holds:*

$$\lim_{\varepsilon \searrow 0} \int_a^b \frac{f(x)}{x \pm \mathrm{i}\varepsilon} \, \mathrm{d}x = \mp \mathrm{i}\pi f(0) + \mathsf{P.V.} \int_a^b \frac{f(x)}{x} \, \mathrm{d}x. \tag{A.1}$$

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