LAMB SHIFT AS A PROBLEM IN MATHEMATICAL PHYSICS

JAN DEREZIŃSKI

Dept. of Math. Methods in Phys.

FACULTY OF PHYSICS

UNIVERSITY OF WARSAW

Quantum Electrodynamics is an extremely successful physical theory, in spite of its mathematical problems. Its perturbative predictions agree with experimental values in a spectacular way. They are, perhaps, one of the greatest achievements of human science.

The famous example is the anomalous magnetic moment of the electron:

$$g_{\rm e} = 2.00231930436118(26) \quad \text{experiment (Gabrielse et al, 2023);}$$

$$g_{\rm e} = 2.00231930436092(43)(5) \quad \text{theory (the first bracket is the uncertainty}$$

of the finestructure constant, the second –theoretical uncertainty (difference between 5-loop contribution according to Volkov and Kinoshita).

$g_{\rm e}$ has a rather clean and well-understood perturbative expansion (it follows from scattering of free electrons in an external magnetic field).

Another great success of QED is the precise computation of bound state energies. Their real part gives the famous Lamb shift.

Here the theoretical problem is polluted by effects from outside of QED: the finite radius of the nucleus, weak and strong interactions. I will say more about the comparison of theory and experiment at the end of my talk.

Theoretical (perturbative) derivation of bound state energies in QED is much more intricate than that of the magnetic moment. In my opinion, this derivation is not understood in a satisfactory way. I would like to formulate it as a rigorous mathematical question.

I am not a professional in this subject, just a dillettante. However, I know a few specialists, and I coorganized a small workshop in the Institute Henri Poincaré in 2013 on this topic. We were asked to organize a panel discussion. I will start with my recollections of this discussion.

Mathematical Challenges of Quantum Electrodynamics

Institute Henri Poincare, Paris

Jan Dereziński, Dept. Math. Meth. In Phys.
University of Warsaw

Krzysztof Pachucki, Inst. Theor. Phys.
University of Warsaw

Paul Indelicato,
Vice-President Recherche et Innovation
Universite Pierre et Marie Curie

Bogumił Jeziorski

Chemistry Dept.
University of Warsaw

Maria Esteban

Ceremade
Universite Paris Dauphine

Vladimir Shabaev

Division of Quantum Mechanics
Saint-Petersburg State University

"BUT THERE IS NO HAMILTONIAN"

According to Quantum Mechanics, a physical system is described by a Hilbert space with a distinguished self-adjoint operator called Hamiltonian that generates the dynamics.

QED is a quantum theory, so one could expect this kind of a description. Unfortunately, it is difficult to find a well-defined Hilbert space and a Hamiltonian in textbooks on QED, or more generally, on Quantum Field Theory. So what is the main object of QFT if it is not a Hamiltonian? Most textbooks are not very clear about this point.

One possible answer, stated eg. in Itzykson-Zuber, is the following: it is the collection of time-ordered n-point vacuum correlation functions.

Why Hamiltonians are not good?

Suppose a physical system is described by a (huge) Hilbert space $\mathcal{H}$. The dynamics is described by a (poorly known) Hamiltonian H. Inside $\mathcal{H}$ we have a (relatively small) subspace $\mathcal{H}_0$, which is well understood. We can write

$$H = \begin{bmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{bmatrix}.$$

Suppose that the initial state belongs to $\mathcal{H}_0$ and we can measure the final state if it falls into $\mathcal{H}_0$. The probability of a measurement is the square of the absolute value of the corresponding amplitude:

$$(\Psi_+ | \mathrm{e}^{-\mathrm{i}tH} \Psi_-), \quad \Psi_+, \Psi_- \in \mathcal{H}_0.$$

Measurable quantities can be described by the Laplace transform of the expectation values

$$-\mathrm{i}\int_0^\infty (\Psi_+|\mathrm{e}^{-\mathrm{i}tH}\Psi_-)\mathrm{e}^{\mathrm{i}tE}\mathrm{d}t \;=\; \big(\Psi_+|(E\mathbb{1}-H)^{-1}\Psi_-\big).$$

where $\mathrm{Im}E > 0$.

Now, by the (Feshbach-)Schur formula

$$\big(\Psi_+|(E\mathbb{1}-H)^{-1}\Psi_-\big) \;=\; \big(\Psi_+|(E\mathbb{1}_0-H_{\mathrm{eff}}(E))^{-1}\Psi_-\big), \qquad (1)$$

where

$$H_{\mathrm{eff}}(E) := H_{00} - H_{01}(E\mathbb{1}_1 - H_{11})^{-1}H_{10}.$$

Thus complete physical information about the subsystem $\mathcal{H}_0$ is contained not in an energy-dependent dissipative effective Hamiltonian $E \mapsto H(E)$. We do not need to know whether it is derived from a self-adjoint Hamiltonian on a bigger space!

Assume that the spectrum of (the big) H is absolutely continuous. Then the effective Hamiltonian can often be extended in E to the real axis, so that

$$\frac{1}{\mathrm{i}}\big(H_{\mathrm{eff}}(E+\mathrm{i}0) - H_{\mathrm{eff}}(E+\mathrm{i}0)^*\big) \leq 0, \quad E \in \mathbb{R}.$$

Often it can be even extended below the real axis, to the non-physical sheet of the complex plane. Its singularities will be called bound state energies. Typically they have a negative imaginary part.

Why time-ordered correlation functions are good?

Suppose that Ω is the ground state of H and

$$\phi[f] = \int \phi(\xi) f(\xi) \mathrm{d}\xi$$

is a family of auxiliary operators called fields, which for simplicity we assume to be self-adjoint. We will write

$$\phi[t, f] := \mathrm{e}^{\mathrm{i}tH} \phi[f] \mathrm{e}^{-\mathrm{i}tH} = \int \phi(t, \xi) f(\xi) \mathrm{d}\xi$$

for these operators in the Heisenberg picture.

The time-ordered correlation functions (also called Green functions) are defined as

$$\Big(\Omega\Big|\mathrm{T}\big(\phi(t_n,\xi_n)\cdots\phi(t_1,\xi_1)\big)\Omega\Big)$$

They are often measurable!

Indeed, suppose the experimentalist can prepare the state Ω in distant past, and he/she can measure Ω in distant future. We also suppose that he/she can perturb the dynamics in a controllable way by adding to the Hamiltonian a field, so that the dynamics is generated by

$$H[f] := H + \phi[f].$$

Thus the resulting amplitude

$$\begin{aligned}
&\lim_{t^+,-t^-\to\infty}\left(\Omega\Big|\mathrm{Texp}\Big(-\mathrm{i}\int_{t^-}^{t^+}H[f(t)]\mathrm{d}t\Big)\Omega\right)\\
=&\left(\Omega\Big|\mathrm{Texp}\Big(-\mathrm{i}\int_{-\infty}^{\infty}\phi[t,f(t)]\mathrm{d}t\Big)\Omega\right)\\
=&\sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int\cdots\int\Big(\Omega\Big|\mathrm{T}\big(\phi(t_n,\xi_n)\cdots\phi(t_1,\xi_1)\big)\Omega\Big)\\
&\qquad\times f(t_n,\xi_n)\cdots f(t_1,\xi_n)\mathrm{d}t_n\mathrm{d}\xi_n\cdots\mathrm{d}t_1\mathrm{d}\xi_1
\end{aligned}$$

is expressed in terms of time-ordered correlation functions.

Two-times Green functions

One can also consider a slightly different picture of a realistic experiment. Let us assume that the space of experimentally accessible states $\mathcal{H}_0$ have the form

$$\Psi_F := \int \int \cdots \int F(\xi_n \ldots, \xi_1)\phi(\xi_n) \cdots \phi(\xi_1)\Omega \mathrm{d}\xi_n \cdots \xi_1$$

for some fixed values of n and some space of functions F. The corresponding amplitudes

$$\begin{aligned}
&\left(\Psi_{F^+}\middle|\mathrm{e}^{-\mathrm{i}(t^+-t^-)H}\Psi_{F^-}\right) \\
&= \int \cdots \int \mathrm{d}\xi_1^+ \cdots \mathrm{d}\xi_1^- \overline{F^+(\xi_{n^+}^+, \ldots, \xi_1^+)} F^-(\xi_{n^-}^-, \ldots, \xi_1^-) \\
&\times \left(\Omega\middle|\phi(t^+, \xi_1^+) \cdots \phi(t^+, \xi_{n^+}^+)\phi(t^-, \xi_{n-}^-) \cdots \phi(t^-, \xi_1^-)\Omega\right)
\end{aligned}$$

are expressed in terms of two-times Green functions.

Taking the Laplace transform of two-times Green functions wrt $t = t^+ - t^-$ we obtain the effective Hamiltonian:

$$\Big(\Psi_{F^+}\Big|\big(E - H_{\rm eff}(E)\big)^{-1}\Psi_{F^-}\Big).$$

Clearly, two-times Green functions can be obtained as limits of the usual time-ordered Green functions.

$$\begin{aligned}
&\Big(\Omega\Big|\phi(t^+,\xi_1^+)\cdots\phi(t^+,\xi_{n^+}^+)\phi(t^-,\xi_{n-}^-)\cdots\phi(t^-,\xi_1^-)\Omega\Big)\\
&= \lim_{\epsilon\searrow 0}\Big(\Omega\Big|\mathrm{T}\big(\phi(t_{1,\epsilon}^+,\xi_1^+)\cdots\phi(t_{n^+,\epsilon}^+,\xi_{n^+}^+)\phi(t_{n^-,\epsilon}^-,\xi_{n-}^-)\cdots\phi(t_{1,\epsilon}^-,\xi_1^-)\big)\Omega\Big),
\end{aligned}$$

$$t_{j,\epsilon}^+ := t^+ + \epsilon(n-j), \qquad t_{j,\epsilon}^- := t^- - (n-j)\epsilon.$$

Quantum Electrodynamics

QED is a perturbative theory of charged particles interacting with (massless) photons. By Furry's Theorem, QED amplitudes without external photons depend only on even powers of e. Therefore, in practice instead of e one uses the finestructure constant $\alpha = \frac{e^2}{4\pi\hbar c}$.

We will always assume that charged particles are massive. One can also assume that photons have a (small) mass μ. Then, to my understanding QED rigorously produces a formal power series in α for renormalized Green functions, uniquely fixed by the physical masses of all particles and their charges. In addition, for charged bosons one needs to put a condition on the value of 4-point function. (One should apply the Bogoliubov-Parasiuk-Hepp-Zimmermann renormalization scheme with the photon propagator in the Feynman gauge. Alternatively, one can define it by renormalization flow equations à la Polchinski).

Because of the infrared problem only selected quantities, called infrared safe have a limit as the photon mass μ goes to zero. One can expect that bound state energies are among them.

The usual approach uses e (or, equivalently, α) as the small parameter. It allows us to compute e.g. inclusive scattering cross-sections of various processes involving free particles. This is described in every textbook,

The theory with $e = 0$ corresponds to noninteracting charged particles and photons. We will not see bound states in the perturbative treatment. This is not surprising: in the usual Quantum Mechanical N-body problem the situation is analogous.

Fortunately, there are at least two approaches, where bound states can be seen already at the zeroth approximation.

QED in external potentials

Suppose that some of the particles are so heavy, that they can be treated just as the sources of the electromagnetic field moving along prescribed trajectories. Then we can use QED with both external and quantized electromagnetic potentials. In the Lagrangian for charged particles we replace eA_μ with $eA_\mu + A_\mu^{\rm ext}$, where $A_\mu^{\rm ext}$ is a prescribed function on spacetime. (Note that there is no small constant e in front of $A_\mu^{\rm ext}$).

Setting $e = 0$, beside independent photons, we obtain independent charged particles in an external potential. The theory of charged particles is quadratic, and hence well understood nonperturbatively. In principle their Green functions are well defined.

If $A_\mu^{\rm ext}$ is stationary, singularities of Green functions correspond to bound states of the (one-body) Dirac/Klein-Gordon Hamiltonian.

Then one can again use e (or α) as the small parameter to add radiative corrections.

This approach is used most often to take into account the potential $\frac{Z\alpha}{|\vec{x}|}$ generated by the nucleus, especially in heavily charged ions such as Uranium, for which $Z\alpha$ is not a small parameter.

Mathematical problem: Does this method yield a systematic algorithm for the bound state energy as a (formal and probably divergent) power series in α and $\ln \alpha$? If so, describe this algorithm. If not, at which order it breaks down?

Note that above a certain order (6?) this is perhaps an academic question, irrelevant for, say, Hydrogen, because pure QED is polluted by effects of a finite size of the nucleus, weak interactions, etc.

Nonrelativistic limit of QED

In the nonrelativistic limit of QED we expect to obtain the many-body Schrödinger-Coulomb Hamiltonian of several species of particles. Photons are not in the picture any more.

For each bosonic "relativistic species", we have two "nonrelativistic species" corresponding to particles and antiparticles, which in the fermionic case have spin $\frac{1}{2}$.

The Hamiltonian is the sum of kinetic terms and 2-body interaction terms. For every species p the kinetic term is

$$\frac{1}{2m_p}\int \mathrm{d}\vec{x} a_p^*(\vec{x})(-\Delta)a_p(\vec{x})$$

For every pair of species $p \neq q$ the interaction term is

$$\frac{1}{2}\int \mathrm{d}\vec{x}\int \mathrm{d}\vec{y} a_p^*(\vec{x})a_q^*(\vec{y})\frac{\alpha z_p z_q \mathrm{e}^{-\mu|\vec{x}-\vec{y}|}}{|\vec{x}-\vec{y}|}a_q(\vec{y})a_p(\vec{x}).$$

Clearly, the many-body Schrödinger-Coulomb Hamiltonian is a well defined self-adjoint operator. Its Green functions are well defined nonperturbatively and one can study rigorously their singularities. They correspond to true bound states and metastable states (resonances) of N-body subsystems.

It is possible (although not easy) to treat Schrödinger-Coulomb Green functions as the zeroth approximation to QED Green functions. One can use $\frac{1}{c}$, or equivalently α, as the small parameter. e is kept constant.

One can also often treat $\frac{m}{M}$ as a small parameter.

This approach is applicable only to systems with small charges. For practical reasons, one usually treats only few particle systems. Typical applications include

1. positronium,
2. Hydrogen with nucleus of finite mass,
3. Helium.

Mathematical problem: Similarly as previously, does this method yield a systematic algorithm for the bound state energy as a power series in α and $\ln \alpha$?

The two lowest levels of Hydrogen are $1s$ and $1p_{\frac{1}{2}}$. According to the Dirac equation they should coincide. QED corrections make them sligthly different. This difference (or actually the main part of it) is called the Lamb shift.

The sharpness of energy levels is limited by various effects. One of them is the natural breadth of the lines. Another is the hyperfine splitting due to the magnetic momentum of the nucleus. The latter is taken into account by a weighted average of all relevant levels. There are also problems due to various non-QED contributions. One of them is the radius of the proton—this has been measured recently independently with the help of muonic atoms.

Here are the relatively recent values of the Lamb shift:

1057.8298(32) MHz — experiment (Hessels et al, 2019)

1057.83412(23)(13) MHz — theory (Yerokhin, Pachucki, Patkóš, 2018)

The first bracket is the uncertainty within QED, the second bracket is non-QED uncertainty. New unpublished results of Yerokhin decrease the first bracket.

THAN YOU FOR YOUR ATTENTION