Part III

Quantum Electrodynamics and Beyond

The Bound State Problem in QED*

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I. Introduction.

In ordinary quantum mechanics there is a Hamiltonian H and one tries to solve the corresponding Schrödinger eigenvalue equation

$$H\,|\mathrm{n}\rangle = E_n\,|\mathrm{n}\rangle\ , \tag{1}$$

where the notation for the case of discrete eigenvalues is used. From the full knowledge of eigenvalues E_n and eigenstates $|\mathrm{n}\rangle$ one can then construct the Green function

$$G = i\sum_n \frac{|\mathrm{n}\rangle\langle\mathrm{n}|}{E-E_n+i\varepsilon}\ . \tag{2}$$

In most cases H is too complicated and eq. (2) cannot be solved in closed form. If one writes

$$H_1 = H + V, \tag{3}$$

where H is a simpler Hamiltonian, whose solutions are supposed to be known, and V a perturbation which is small compared to H, standard perturbation theory can be used to get the eigenvalues $E_n^{(1)}$ of H_1 in the customary form

$$E_n^{(1)} = E_n + \langle V\rangle_n + \cdots. \tag{4}$$

Similarly, the Green function for the Hamiltonian (3) becomes

$$G^{(1)} = G + GVG + \cdots. \tag{5}$$

In QED the situation is quite different. The starting point for the Coulomb bound state problem is the (renormalized) perturbative expansion in the fine structure constant $\alpha \approx 1/137$ of the Green function for the relevant two body scattering problem (μ^+e^- scattering for muonium, the μ^+e^- bound state, etc.),

$$G = \sum_{n=0}^{\infty}\left(\frac{\alpha}{\pi}\right)^n G^{(n)}, \tag{6}$$

where the $G^{(n)}$ are sums of the renormalized off mass–shell Feynman graphs for that scattering process. The kernel for the expansion (6) is then defined as

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(7) $$K = G_0^{-1} - G^{-1} \ ,$$

where G_0 is a zeroth order Green function for the problem. If G_0 is the product of the free propagators of the two scattering particles, then, since G and G^{-1} are (formal) power series in $\left(\frac{\alpha}{\pi}\right)$, K itself can also be obtained as a (formal) power series in $\left(\frac{\alpha}{\pi}\right)$:

(8) $$K = \sum_{n=0}^{\infty} \left(\frac{\alpha}{\pi}\right)^n K^{(n)}.$$

Combinatorics shows that K is the sum of all two-fermion irreducible graphs.

From (7) one obtains the Bethe-Salpeter equation

(9) $$G = G_0 + G_0 K G \ ;$$

the corresponding equations for the wave function and its conjugate are

(10) $$\begin{cases} \psi_n = G_0 K \psi_n \, , \\ \bar{\psi}_n = \bar{\psi}_n K G_0 \ . \end{cases}$$

Note that according to eq. (7), eq. (9) is true almost by definition; its justification derives from the fact that by trivial perturbative iteration it reproduces the (formal) expansion eq. (6). The kernel, as defined through eq. (7), plays the role of the interaction in that approach. With respect to ordinary quantum mechanics the situation is therefore almost reversed. The Green function eq. (6) is known and the kernel is obtained from it; the problem is that the (formal) expansion eq. (6) does not exhibit a bound state at any order in α; eqs. (7),(8),(9) are then used as a guideline for a suitable resummation of (6). The kernel is an infinite (formal) series in itself that depends explicitly on the energy. An exact solution of eq. (9) in closed form is obviously out of reach; it is almost mandatory to pick up a leading Coulomb kernel K_c and a perturbation kernel δK defined by

(11) $$K = K_c + \delta K \ ,$$

where δK is again a power series in $\left(\frac{\alpha}{\pi}\right)$. Then one can consider the lowest order equation

(12) $$G_c = G_0 + G_0 K_c G_c \ ;$$

the solution of (12) gives the unperturbed bound state energy levels as the position E_n^c of its singularity in the complex energy plane and the corresponding wavefunctions are obtained from the residues. Standard perturbation theory then gives the corrections to the energy levels

(13) $$E_n = E_n^c + \langle \delta K \rangle_n + \langle \delta K \hat{G}_c \delta K \rangle_n + \langle \delta K \rangle_n \langle \delta K' \rangle_n + \cdots \ ,$$

where $\hat{G}_c$ is equal to G_c without the nth pole, $\delta K'$ is the derivative of δK with respect to the energy and $\langle \rangle_n$ is the average over the nth wave function. The expansion (13) can then be rearranged as a series in $\left(\frac{\alpha}{\pi}\right)$.

It took some time to invent a suitable way of writing a Coulomb kernel K_c for which a solution in closed form can be derived[1]. Most of the results which were found so far in bound state calculations, have indeed been obtained with very little or no direct use of the formalism sketched above. In hydrogen and $\mu^+ e^-$, e. g., it is natural to expand in the ratio of the masses of the electron and the positive particle and therefore to use a simplified formalism from the beginning. In positronium, however, the masses of the constituents are

equal and simple approximations are not adequate (see, however, the recent approach by Caswell and Lepage[2] who propose an interesting way to circumvent the Bethe–Salpeter covariant formalism in favor of a purely nonrelativistic treatment).

II. Brief Review of Results.

Not very much has changed since the 1984 Washington conference on Atomic Physics, to which we refer for further details[3].

i. Hydrogen Lamb Shift. Historically this is the first bound state problem which was attacked while the foundations of QED were at the same time being laid. In most of the classical results the proton can be regarded as an external field and one deals with mean values of relativistic electron self mass radiative corrections averaged over the nonrelativistic Schrödinger wave function. Unfortunately the accuracy of Lamb shift results is, by present standards, very limited for both experimental and theoretical reasons: the natural line width of the $2P_{1/2}$ state (about 100MHz) makes it almost impossible to measure the 1.058 GHz of the Lamb shift to better than 10 ppm or 10 kHz and the contribution of proton structure (finite size) effects has a $7\approx10$ kHz error which theory cannot compute.

ii. H hyperfine splitting. A similar situation occurs in the H hfs. Here the experimental results are extremely good (with a relative error of 10^{-13}) but again proton finite size effects spoil the theoretical prediction at the 1 ppm level.

iii. Muonium hyperfine splitting. No theoretical limitations are present to μ^+e^- which can, in principle, be evaluated to any desired accuracy. Indeed the precision of the theoretical prediction is very good, 0.5 ppm. The bound state part of the problem is greatly simplified by an expansion in $\frac{m_e}{m_\mu}$ (as well as in α). $O(\alpha^2)$ and $O(\alpha\frac{m_e}{m_\mu})$ corrections are known and only some $O(\alpha^3)$ corrections remain to be calculated. Unfortunately, because of this dependence on $\frac{m_e}{m_\mu}$ besides the Rydberg constant and α, the muonium hfs is used to obtain a more accurate value for this ratio rather than being a stringent test of QED or an independent, precise determination of α. An update on these results can be found in ref[4].

III. Positronium.

As for muonium, no a priori limitations prevent positronium from being used as an accurate test of bound state QED; in practice, however, there are serious difficulties to surmount before a competitive level of precision can be reached. The system is indeed so light that Doppler broadening and similar effects are experimentally particularly difficult to control, while on the theoretical side calculations are an order of magnitude harder than for the previously discussed systems. The most accurate prediction is in fact currently the ground state hfs:

$$\Delta\nu(\text{hfs,th}) = \text{Ry}\,\alpha^2\left[\frac{7}{6} - \left(\frac{\alpha}{\pi}\right)\left(\frac{16}{9} + \ln 2\right) - \frac{5}{12}\alpha^2\ln\alpha\right], \tag{15}$$

where the $O(\alpha^2)$ corrections are still to be calculated.

Another important problem which has always been around has recently acquired new importance: the decay rates. New experimental results from 1987[5]:

$$\Gamma(3\gamma,\text{exp}) = 7.0516(13)\times 10^6 s^{-1} \tag{16}$$

showed a 10σ(exp) disagreement with the theoretical prediction, lowest order plus one–loop $\left(\frac{\alpha}{\pi}\right)$ corrections[6]:

$$\Gamma(3\gamma,\mathrm{th}) = \frac{2}{9\pi}(\pi^2-9)m\alpha^6 \times \left\{1 - 10.282(3) \times \left(\frac{\alpha}{\pi}\right)\right\} \approx 7.0389 \times 10^6 s^{-1} \,. \tag{17}$$

In order to recover agreement between theory and experiment, one needs either a value of about $-9\left(\frac{\alpha}{\pi}\right)$ for the first order correction, i. e. a difference of $+1 \times \left(\frac{\alpha}{\pi}\right)$ with respect to the reported value $-10.3 \times \left(\frac{\alpha}{\pi}\right)$, or an extremely large $O\left(\frac{\alpha}{\pi}\right)^2$ term.

In an attempt to understand whether the discrepancy might be due to a theoretical error, we have carried out an ab initio recalculation of the one–loop correction to the decay rate using the full Bethe–Salpeter formalism of ref.[1] and exercising particular care in studying the approximations that are anyhow needed in the calculation. To focus attention on binding problems, we considered the simpler case of para–positronium (which is less well known experimentally). It is obvious that most of the following discussion applies to ortho–positronium as well. We have used Feynman gauge throughout.

Quite in general, decay rates are the imaginary parts of radiative energy shifts; the lowest order kernel $\delta K^{(2)}$ contributing to para–Ps decay is depicted in Fig.1:

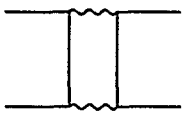


Fig. 1: The lowest order kernel $\delta K^{(2)}$ for parapositronium decay.

Following reference[1] we use the wave function

$$\psi(W_0,p_0,\mathbf{p}) = \frac{i}{E_\mathbf{p}}\left[E_\mathbf{p} + (m - \vec{\mathbf{p}}\cdot\vec{\gamma})\gamma_0\right]\gamma_5 \frac{(E_\mathbf{p}-W_0)\sqrt{E_\mathbf{p}+W_0}}{p_0^2-(E_\mathbf{p}-W_0)^2+i\varepsilon} \times \phi(\mathbf{p}), \tag{18}$$

where

$$\phi(\mathbf{p}) = \frac{8\pi\gamma}{(\mathbf{p}^2+\gamma^2)^2}\sqrt{\frac{\gamma^3}{\pi}}, \tag{19}$$

with the notation

$$\gamma = \frac{m\alpha}{2}\,, \qquad W_0 = \sqrt{m^2-\gamma^2}\,, \tag{20}$$

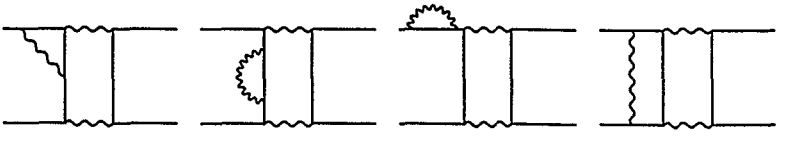
is the nonrelativistic Schrödinger wave function. As the very first step, we integrate on the relative energy p_0, then on $\mathbf{p}$. The contribution corresponding to Fig.1 is found to be

$$\Gamma^{(2)} = \langle \delta K^{(2)} \rangle = \Gamma_0 \cdot \left\{1 + 2a_0\left(\frac{\alpha}{\pi}\right)\right\}, \tag{21}$$

where

$$\Gamma_0 = \frac{1}{2}m\alpha^5 \tag{22}$$

is the lowest order decay rate, well known in the literature. For the coefficient of the $O\left(\frac{\alpha}{\pi}\right)$ correction in (21), we find $a_0 = -3.1137...$; its explicit value is, however, somewhat irrelevant, as it is found to be reabsorbed by the one-loop contributions to be discussed below.



δK_a δK_b δK_c δK_d

Fig. 2: Next to leading order kernels for parapositronium decay.

The kernels contributing to next to leading order in $\left(\frac{\alpha}{\pi}\right)$ are usually depicted as in Fig. 2; they contribute to the actual decay rate with multiplicities 2,4,2,2 respectively. Kernels $\delta K_{a,b,c}$ are UV divergent; to evaluate them we use a Pauli–Villars regulator with square mass A and then perform on–shell mass renormalization; we do not carry out on–shell wave-function and vertex renormalization because on the one hand that would introduce spurious IR divergences while, on the other hand, those remaining UV divergences cancel out in the sum anyhow.

We find

$$\Gamma_a = \langle \delta K_a \rangle = \Gamma_0 \left(\frac{\alpha}{\pi}\right) \left(-\frac{1}{4}\ln A + 2\ln 2 - \frac{5}{8}\right) , \tag{23}$$

$$\Gamma_b = \langle \delta K_b \rangle = \Gamma_0 \left(\frac{\alpha}{\pi}\right) \left(\frac{1}{4}\ln A - \ln 2 + \frac{\pi^2}{16} + \frac{1}{8}\right) , \tag{24}$$

so that

$$\Gamma_a + \Gamma_b = \langle \delta K_a \rangle + \langle \delta K_b \rangle = \Gamma_0 \left(\frac{\alpha}{\pi}\right) \left(\frac{\pi^2}{16} + \ln 2 - \frac{1}{2}\right) ; \tag{25}$$

which is finite and in full agreement with all previous calculations (note, however, that δK_a and δK_b contribute to the actual rate in a different combination).

Kernels c–d are not two–fermion irreducible; strictly speaking they enter in the calculation through the term of second order in δK of eq. (13) where $\hat{G}_c$ is approximated by the free two–fermion propagator and the two irreducible irreducible kernels are: self–mass and lowest order two–photon annihilation in δK_c, one–photon exchange and again $\delta K^{(2)}$ in δK_d. With the already discussed regularization we find

$$\langle \delta K_c \rangle = \Gamma_0 \left(\frac{\alpha}{\pi}\right) \left(-\frac{1}{4}\ln A - 2\ln \alpha - \ln 2 - \frac{9}{8}\right) . \tag{26}$$

Note the presence of the IR divergence which is naturally parametrized by $\ln \alpha$ when the proper wave function eq. (18) is used.

The last term, $\langle \delta K_d \rangle$, is also referred to as the binding diagram. It involves the one–photon exchange which, however, contains the binding kernel K_c. According to eq. (11) the proper kernel to be used, which we call δK_f, can be depicted as in Fig. 3, as the difference between the full photon exchange and K_c.
The correct contribution from δK_d is then

$$\begin{aligned} \Gamma_d &= \langle \delta K_f G_0 \delta K^{(2)} \rangle \;=\; \langle \delta K_d \rangle \;-\; \langle K_c G_0 \delta K^{(2)} \rangle \\ &= \langle \delta K_d \rangle \;-\; \langle \delta K^{(2)} \rangle \end{aligned} , \tag{27}$$

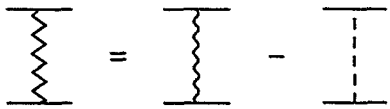


Fig. 3: δK_f expressed as the difference between the full–photon exchange and K_c.

where use has been made of eq. (10). Explicit calculation gives

$$\langle \delta K_d \rangle = \Gamma_0 \cdot \left[1 + a_0 \left(\frac{\alpha}{\pi}\right)\right] \left\{ \frac{\sqrt{2}}{\pi^2}\gamma^2 \cdot \int \mathrm{dp} \frac{\mathrm{p}}{(\mathrm{p}^2+\gamma^2)^2} \frac{\sqrt{\mathrm{E_p}+\mathrm{W_0}}}{\mathrm{W_0 E_p}} (2\mathrm{W_0 E_p} - 1) \right.$$

$$\times \int \frac{\mathrm{dk}}{\mathrm{E_k}} \frac{1}{\mathrm{E_k} - \mathrm{W_0}} \ln \frac{\mathrm{E_k}+\mathrm{k}}{\mathrm{E_k}-\mathrm{k}} \ln \frac{\mathrm{E_p}-\mathrm{W_0}+\mathrm{E_k}-\mathrm{W_0}+\mathrm{p}+\mathrm{k}}{\mathrm{E_p}-\mathrm{W_0}+\mathrm{E_k}-\mathrm{W_0}+|\mathrm{p}-\mathrm{k}|} \tag{28}$$

$$\left. + \left(\frac{\alpha}{\pi}\right)\left(\ln 2 - \frac{1}{2}\right)\right\} \; - \langle \delta K^{(2)} \rangle$$

$$= \Gamma_0 \cdot \left\{1 + a_0 \left(\frac{\alpha}{\pi}\right) + \left(\frac{\alpha}{\pi}\right)(3\ln\alpha + \ln 2 - 1)\right\} \; - \langle \delta K^{(2)} \rangle \; .$$

Note the appearance of a_0, already introduced in eq. (21). It is to be observed that δK_d has an IR divergence as well.

Summing up these results, one finds

$$\begin{aligned} \Gamma =& \Gamma^{(2)} + 2\left(\Gamma_a + 2\Gamma_b + \Gamma_c + \Gamma_d\right) \\ =& \Gamma_0 \left\{1 + \left(\frac{\alpha}{\pi}\right)\left(2\ln\alpha + \frac{\pi^2}{4} - 5\right)\right\} \; . \end{aligned} \tag{29}$$

Such a result is somewhat surprising since it contains an unexpected — and undesired — $\ln\alpha$ term. Eq. (28) cannot be directly compared with previous calculations, as their form depends on the way UV and IR divergences are parametrized.

When using the wave function eq. (18) the decay kernels of fig. (2) are to be evaluated for incoming fermion four momenta $(\mathrm{p_0}+\mathrm{W_0}, \vec{\mathrm{p}})$, $(\mathrm{p_0}-\mathrm{W_0}, \vec{\mathrm{p}})$; we found, however, that if we neglect the p_0–dependence in the kernels, which amounts to disregarding $(\mathrm{E_p}-\mathrm{W_0})$ in eq. (29), our results change into

$$\langle \delta K_c \rangle = \Gamma_0 \left(\frac{\alpha}{\pi}\right)\left(-\frac{1}{4}\ln A - 2\ln\alpha - \frac{9}{8}\right) \; , \tag{30}$$

$$\langle \delta K_d \rangle = \Gamma_0 \left\{1 + a_0\left(\frac{\alpha}{\pi}\right) + \left(\frac{\alpha}{\pi}\right)(2\ln\alpha - 1)\right\} - \langle \delta K^{(2)} \rangle \; , \tag{31}$$

giving

$$\Gamma = \Gamma_0 \left\{1 + \left(\frac{\alpha}{\pi}\right)\left(\frac{\pi^2}{4} - 5\right)\right\} \; , \tag{32}$$

which is the old result of Harris and Brown[7] that has been reproduced in all subsequent calculations. This result is, to $\mathrm{O}\left(\frac{\alpha}{\pi}\right)$, not affected by the replacement $\sqrt{\mathrm{E_p}+\mathrm{W_0}} \to \sqrt{2m}$ in eq. (28).

Clearly the situation is confused. The p_0–dependence is there, both in the wave function and kernels and a systematic approach cannot simply ignore it. While it is true that p_0 is in some sense of $O(\alpha^2)$ in the calculation, it can nevertheless contribute an $\alpha \ln \alpha$ as we have shown explicitly. On the other hand, if we accept that no $O(\alpha \ln \alpha)$ term is present in the final result, additional contributions from higher order terms must exist, which compensate the unwanted $\alpha \ln \alpha$ and give, presumably, additional $O\left(\frac{\alpha}{\pi}\right)$ terms as well. It is indeed not difficult to find two–loop candidates for $O\left(\frac{\alpha}{\pi}\right)$ corrections; the replacement of $\hat{G}_c$ with G_0 should also be considered more carefully.

As a last remark, we mention that we have used Feynman gauge throughout, although it is common wisdom that the use of Coulomb gauge usually results in faster convergence for bound state problems. It is to be observed, however, that Coulomb gauge can cause additional problems in positronium as binding photons and photons giving rise to UV divergences mix so that one has to either renormalize everything in Coulomb gauge or one needs to rely on problematic mixed gauge prescriptions. But, as the last remark, we point out that the discrepancy between eqs. (29) and (32) is not due to the use of different gauges as eq. (32) has also been obtained in ref.[7] and by subsequent authors in Feynman gauge as well.

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