QED on background Coulomb field

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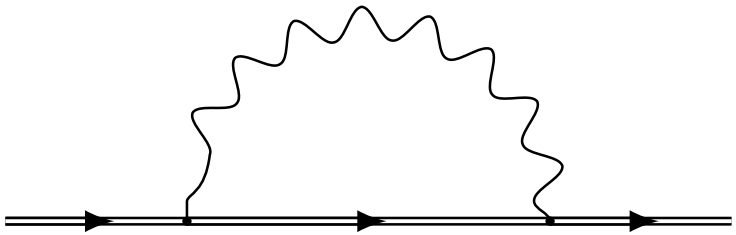
May 2017

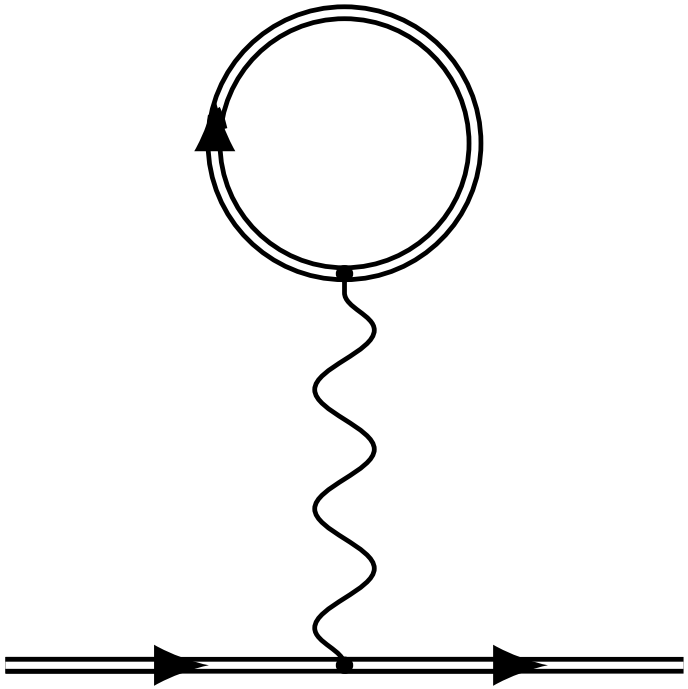
Plan of the talk

- Motivation for study bound-state QED
- Solution of Dirac equation for external Coulomb field
- Evaluation of the self-energy effect



Plan of the talk

- Evaluation of the vacuum polarization effect



Motivation for study of bound-state QED

- Practical - determination of nuclear properties (proton radius, etc.)
- Conceptual -
  - QFT is the theory of almost everything
  - Study of perturbative aspects have been bringing continual surprises, even in the last few years (helicity spinors, twistors, unitary method, finitness of the first four orders of $N = 8$ supergravity, etc.)
  - Study of non-perturbative aspects still in infancy, but for example Higgs boson is very likely associated with them, not to say about quark confinement, etc.
  - Bound-state QED is the simplest, and yet very useful, example of non-perturbative problem

Solution of Dirac equation for external Coulomb field

The Dirac equation:

$$(\gamma.\Pi - m)\psi = 0$$

By multiplying the Dirac equation by $\gamma.\Pi + m$ we get

$$H\psi = 0\,, \quad H = \Pi.\Pi - m^2 + \frac{1}{4}[\Pi_\mu, \Pi_\nu][\gamma_\mu, \gamma_\nu].$$

For Coulomb external field $\Pi = \left(E + \frac{Z\alpha}{r}, \vec{p}\right)$ and after scaling $r \to \frac{r}{EZ\alpha}$

$$H_l = E^2 - m^2 - 2(EZ\alpha)^2 \left[\frac{1}{2}\left(p_r^2 + \frac{l(l+1)}{r^2}\right) - \frac{1}{r}\right].$$

where $l(l+1)$ is an eigenvalue of the operator $L^2 - i(Z\alpha)\gamma_0\vec{\gamma}.\vec{n} - (Z\alpha)^2$,

$$l = \sqrt{(j+1/2)^2 - (Z\alpha)^2} - \delta_{\rho,1}\,, \quad \rho = \pm 1$$

Advantages of the second-order Dirac Hamiltonian

Spectral decomposition of $f(H_l)$ is of the form

$$f(H_l) = \sum_n f(E_n)|n,l><n,l| + \int_0^\infty dk_e f(E_{k_e})|k_e,l><k_e,l|$$

$$E_{k_e} = (mZ\alpha)^2[1+k_e^2]\,.$$

- Radial and spinor-angular degrees of freedom are separated
- Radial functions are of those of non-relativistic form
- Matrix elements of the bound-bound and bound-continuum transitions (those needed for self-energy calculation) possible to express in closed, compact form through hypergeometric functions
- The same holds for some of the continuum-continuum transitions (those needed for vacuum polarization calculation)

Self-energy – Practical Importance

- The different proton radii $r_p = 0.8768fm$ and $r_p = 0.84184fm$ shift 2s-1s transitions in hydrogen by 1.052 MHz and 0.96977 MHz, respectively.
- The uncertainty in determination of proton charge radius amounts to 82kHz for 2s-1s transition
- One-loop self-energy shifts the transition by about 7.3GHz
- It has to be determined with precision significantly better than 1 part in 10^5 in order to exclude the possibility that the proton charge radius is influenced by error in determination of the self-energy
- Error of perturbative calculation, $Z\alpha$ expansion, (Pachucki 1990) amounts to 24kHz
- Non-perturbative (in $Z\alpha$) treatment necessary even for hydrogen.

Self-energy – (Very) Short History

$Z\alpha$-expansion

$$\Delta E = \frac{m\alpha(Z\alpha)^4}{\pi n^3 s^3} F(Z\alpha, n, l_j)\,, \quad s = 1 + \frac{m}{m_n}$$

where

$$F(Z\alpha, n, l_j) = A_{41} \ln s(Z\alpha)^{-2} + A_{40} + A_{50}(Z\alpha) +$$

$$+(Z\alpha)^2 \left[A_{62} \ln^2 s(Z\alpha)^{-2} + A_{61} \ln s(Z\alpha)^{-2} + A_{60}\right] + \ldots$$

Weiskopf,Bethe,Schwinger,Feynman,Yennie,Pachucki, etc.
The $Z\alpha$ expansion is restricted to low Z only and gives sufficiently accurate results for the non-S-states and the normalised difference of the S-states

$$n^3 \Delta E_n - \Delta E_1$$

but not for the ground state ΔE_1.
1-D integrals numerically

Self-energy – (Very) Short History

Partial wave expansion

$$\Delta E = \langle O - \Delta m \rangle$$

where mass operator O is written as

$$\langle O \rangle = -\frac{\alpha}{\pi} \int_0^{\Lambda^2} d\lambda \int \frac{i dk_0}{(2\pi)^2} \int \frac{d^3k}{(k_0^2 - \omega^2 - \lambda)^2}$$

$$\int d^3\vec{r}_1 d^3\vec{r}_2 \psi^+(\vec{r}_1)\gamma_0\gamma_\mu e^{i\vec{k}.\vec{r}_1} G(-k_0 + E, \vec{r}_1, \vec{r}_2) e^{-i\vec{k}.\vec{r}_2}\gamma_0\gamma_\mu\psi(\vec{r}_2)$$

and $G(z, \vec{r}_1, \vec{r}_2)$ is the Green function of the first-order Dirac Hamilton operator.

The plane waves and the Green function expanded in the partial waves

Mohr, Jentschura, etc.

Works well for large Z and the low lying states

3-D integrals numerically

Self-energy - source of difficulties

Existence of several different scales

- The self-energy represents an 11-D integral; at least one integration has to be done numerically in any method.
- The low-energy photon region $\omega \sim m(Z\alpha)^2$ gives the dominant contribution (Bethe non-relativistic estimate)
- The high-energy photon region $\omega \sim m$ necessary to get renormalization of electron mass correctly
- The low-energy electron region $k_e \sim 1$ contributes to the dominant part of the effect
- The high-energy electron region $k_e \sim (Z\alpha)^{-1}$ yields the subdominant contribution ($Z\alpha$-correction)

Relativistic generalisation of multipole expansion

In our method the renormalized expression for the self-energy

$$\Delta E = \langle O - \Delta m \rangle = < \psi | \gamma_0 (O - \Delta m) | \psi >,$$

with regularized mass operator O defined as

$$O = \frac{\alpha}{\pi} \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2 - \lambda)^2} \gamma_\mu \frac{1}{\gamma.(\Pi - k) - m} \gamma_\mu,$$

is rewritten into second-order form

$$\langle O \rangle = -\frac{\alpha}{2\pi} \left\langle \gamma_\mu \left(G_4 \Pi_\mu - \frac{m}{2} G.\gamma \gamma_\mu \right) \right\rangle$$

with

$$G_{4,\nu} = (-4) \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2 - \lambda)^2} \frac{(1, k_\nu/m)}{k^2 - 2k.\Pi + H}.$$

Relativistic generalisation of multipole expansion

The key idea of our method is that the electron propagator can be expanded in powers of difference of the electron four-momentum Π and the four-momentum of the electron at rest $\varepsilon = (m, \vec{0})$

$$\frac{1}{k^2 - 2k.\Pi + H} = \frac{1}{k^2 - 2k.\varepsilon + H} +$$

$$+ \frac{1}{k^2 - 2k.\varepsilon + H} 2k.(\Pi - \varepsilon) \frac{1}{k^2 - 2k.\varepsilon + H} +$$

$$+ \frac{1}{k^2 - 2k.\varepsilon + H} 2k.(\Pi - \varepsilon) \frac{1}{k^2 - 2k.\varepsilon + H} 2k.(\Pi - \varepsilon) \frac{1}{k^2 - 2k.\varepsilon + H} + \dots .$$

Relativistic generalisation of multipole expansion

Motivation:

- To get correctly Bethe non-relativistic estimate, the second-order hamiltonian H has to be kept at the leading approximation to the propagator.
- The greatest overlap between the reference and the virtual states lies in the region of energies close to the ionisation threshold. The momentum of virtual electron in this region, $p \sim mZ\alpha \Leftrightarrow k_e \sim 1$, is small compared to the rest mass m.

Advantages:

- After renormalization of electron mass is performed all the integrals over both the photon and electron variables are automatically finite both at infrared and ultraviolet.
- Except for the integration over the hydrogen continuous spectrum everything is done analytically, yet non-perturbatively in $Z\alpha$.
- Individual terms of the expansion can be generated automatically using symbolic computer languages.

Relativistic generalisation of multipole expansion

In the case of non-S-states and the normalised difference of the S-states $n^3\Delta E_n - \Delta E_1$ the contribution from the high-energy virtual electron region is suppressed and the RME converges rather fast. Just four terms in the expansion are enough to obtain results that surpass accuracy of the experiment and any other method. Result for $2^3\Delta E_2 - \Delta E_1$:

Term	$Z = 1$	$Z = 5$
$F_1 + F_2$	0.229991606931	0.232342252851
F_3	0.000039870858	0.000884923162
F_4	6.241492×10^{-8}	6.131626×10^{-6}
Total	0.2300315402(3)	0.23323331(3)

V. Patkóš and J. Zamastil, Phys. Rev. A **91**, 062511 (2015).

- The RME method is based on the assumption that the difference $\Pi - \varepsilon$ is small. This assumption holds with the exception for the region of high $k_e \gtrsim (Z\alpha)^{-1}$.
- In order to get accurate results the high energy virtual electron region needs separate treatment.
- The contribution from the high-energy electron region is contained in RME in the form of slowly converging series.
- Fortunately, the most important part, of the order $\alpha(Z\alpha)^5$, can be isolated by taking limit of small $Z\alpha$ and high k_e

$$A_{50}^{(v)} = -2^3 \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(v-\frac{5}{2}\right)\left(16v^4-32v^3+296v^2+8v-267\right)}{\pi\Gamma(v)(2v+5)(2v+3)(2v+1)^2(2v-3)}.$$

- For large v this behaves as $A_{50}^{(v)} \simeq v^{-7/2}$.

- The accuracy of RME can then be improved by subtracting $A_{50}^{(v)}$ and adding the whole A_{50}:

$$F(Z\alpha) = (Z\alpha)A_{50} + \sum_{v=1}^{\infty} S_v\,, \quad S_v = F_v - (Z\alpha)A_{50}^{(v)}.$$

- Here, the total contribution of the order $\alpha(Z\alpha)^5$ is

$$A_{50} = \sum_{v=1}^{\infty} A_{50}^{(v)} = 4\pi\left(\frac{139}{128} - \frac{\ln 2}{2}\right)$$

- This significantly improves accuracy for $Z < 20$.

Results - ground state of hydrogen

lead	10.315870916
S_3	$0.891183\ 10^{-3}$
S_4	$0.23509\ 10^{-4}$
S_5	$0.4484\ 10^{-5}$
S_6	$0.1554\ 10^{-5}$
S_7	$0.719\ 10^{-6}$
S_8	$0.388\ 10^{-6}$
S_9	$0.237\ 10^{-6}$
sum	10.316792992
small	$0.684(7)\ 10^{-6}$
total	10.316793675(7)
PWE	10.316793650(1)

- J. Zamastil, V. Patkóš, Phys. Rev. A 88, 032501 (2013)
- PWE – U. D. Jentschura et al., Phys. Rev. A 63, 042512 (2001), extrapolation of several millions of 3-D integrals

Results - ground state of hydrogen-like ions

The relative difference 2 parts in 10^9 corresponds to 18Hz for $2s - 1s$ transition in hydrogen.
Higher nuclear charges:

Z	RME	PWE
5	6.2516278	6.251627078
10	4.654156	4.6541622
20	3.24618	3.2462556
30	2.5525	2.5520151
40	2.1359	2.1352284
50	1.8646	1.8642743

PWE results for $Z \geq 10$ are from P.J. Mohr, Phys. Rev. A 46, 4421 (1992).

Role of Relativistic Effects

Generic integral encoutered in RME:

$$m\frac{\alpha(Z\alpha)^6}{\pi}C_0\int_0^1 dwf(w)\times \tag{1}$$

$$\times\int_0^1 dyy^u\int_0^\infty dk_e\frac{k_e^{-2l_0}}{y+a(1+k_e^2)}\left(1+\frac{C_1k_e}{1+k_e^2}+\dots\right),$$

$u \geq 0$ depends on the order of RME

C_0 and C_1 are some complicated functions of quantum numbers of intermediate states, pertinent order of RME, etc.

$a = w(Z\alpha)^2$

$f(w)$ is some polynomial function of w

$l_0 = \sqrt{1-(Z\alpha)^2}-1$ enters into Eq. (1) through the overlap integrals between the Dirac ground state wave function of hydrogen $\psi_{1s} \sim \exp\{-r/(l_0+1)\}\, r^{l_0}$ and the wave functions of the hydrogen intermediate states.

Role of Relativistic Effects

$$\Delta E = m\frac{\alpha}{\pi}(Z\alpha)^4 F(Z\alpha)\,,$$

$$F(Z\alpha) = A_{41}\ln(Z\alpha)^{-2} + A_{40} + A_{50}(Z\alpha) +$$

$$+(Z\alpha)^2\left[A_{62}\ln^2(Z\alpha)^{-2} + A_{61}\ln(Z\alpha)^{-2} + G(Z\alpha)\right]$$

$$G(Z\alpha) = A_{60} + (Z\alpha)\left[\ln(Z\alpha)^{-2}A_{71} + A_{70}\right] +$$

$$+(Z\alpha)^2\left[\ln^3(Z\alpha)^{-2}A_{83} + \ln^2(Z\alpha)^{-2}A_{82} + \ln(Z\alpha)^{-2}A_{81} + A_{80}\right] +$$

$$+(Z\alpha)^3\left[\ln^2(Z\alpha)^{-2}A_{92} + \ln(Z\alpha)^{-2}A_{91} + A_{90}\right] + \ldots.$$

$$\frac{A_{71}}{A_{50}} = \frac{1}{2},\ \frac{A_{92}}{A_{50}} = \frac{1}{8},\ \frac{A_{11,3}}{A_{50}} = \frac{1}{48},\ \ldots$$

$$\frac{A_{83}}{A_{62}} = \frac{1}{6},\ \frac{A_{10,4}}{A_{62}} = \frac{1}{48},\ \ldots$$

Role of Relativistic Effects

The first relation appears in S. G. Karshenboim, Z. Phys. D **39**, 109 (1997)
the others in V. Patkóš, D. Šimsa, and J. Zamastil, Phys. Rev. A **95**, 012507 (2017)
NRQED approach (originally proposed by Caswell and Lepage, developed into powerfull method by Pachucki and coworkers)

$$H = m\alpha^2(H_0 + \alpha^2 H^{(4)} + \alpha^3 H^{(5)} + \alpha^4 H^{(6)} + \alpha^5 H^{(7)} + \ldots)$$

has to eventually breaks down: for $\alpha \ln^3(\alpha)^{-2} \simeq 6.95 > 1$. Whence it does not appear meaningful to construct $H^{(8)}$ and completely neglect $H^{(9)}$.

Future developments

- Relativistic multipole expansion – to determine the portion of A_{60} coefficient contained at given order of RME
- Partial wave expansion – by means of the second order Hamiltonian
  - integrals reduced to 2D integrals
  - the mass renormalization can be done exactly
  - A_{40}, A_{41} coefficients included exactly
  - determine the portion of A_{50} coefficient at given order of PWE
- Two loops
  - SEVP graphs – preliminary calculation for muonic hydrogen
    V. Patkóš, D. Šimsa, and J. Zamastil, Phys. Rev. A **95**, 012507 (2017)
    $\Delta E(2p_{\frac{1}{2}}) - \Delta E(2s) \simeq -2.706 \times 10^{-6}\,\mathrm{eV}$
    which differs by 8% from the result $-2.5 \times 10^{-6}\,\mathrm{eV}$,
    U. D. Jentschura, Ann. Phys. **326**, 500 (2011).
  - Double SE graphs – Still lot of work ahead
    the greatest problem with general continuum–continuum transition

Vacuum polarization

Assuming non-relativistic approximation of the bound-state function the energy shift can be expressed through Laplace transform of the vacuum charge density

$$\Delta E = m_r \left(\frac{m_r}{m}\right)^2 \frac{(Z\alpha)^3}{4\pi} \left(-\frac{d}{db}\right) \left[b^{-2} \int_0^b db' q(b')\right]\Big|_{b=\frac{m_r}{m} Z\alpha}$$

$$q(b) = \int d^3\vec{r} \exp\{-2mbr\} e\langle\rho(\vec{r})\rangle$$

$$\langle\rho(\vec{r})\rangle = e \int_C \frac{dE}{2\pi i} \langle\vec{r}|\mathrm{Tr} \frac{1}{E - \hat{V} - \gamma_0\vec{\gamma}\cdot\hat{\vec{p}} - \gamma_0 m}|\vec{r}\rangle =$$

$$= e \int_C \frac{dE}{2\pi i} \langle\vec{r}|\mathrm{Tr}(E - \hat{V} - \gamma_0\vec{\gamma}\cdot\hat{\vec{p}} + \gamma_0 m)\frac{1}{H}|\vec{r}\rangle,$$

Vacuum polarization

$$q(b) = -4\alpha \sum_{k=1}^{\infty} \sum_{\rho=\pm 1} k \int_0^{\infty} dp \int_0^1 \frac{dt}{t(1-t)} \times$$

$$\times \left\{ \left(-\frac{\partial}{\partial b} \right) \frac{b}{2} \sinh\{a(pb)A(p)\} + \right.$$

$$\left. + Z\alpha \left(1 + \frac{b}{2\Gamma} \frac{\partial}{\partial b} \right) \frac{b \cosh\{a(pb)A(p)\}}{\sqrt{(bp)^2+1}} \right\} s^{l+1} ,$$

where

$$l = \sqrt{k^2 - (Z\alpha)^2} - \delta_{\rho,1}$$

$$a(pb) = \frac{\sqrt{(bp)^2+1}}{bp} Z\alpha, \; A(p) = \pi - 2\arctan(p) + i \ln \left(\frac{1-t}{t[1-tz(p)]} \right)$$

and

$$z(p) = \frac{p^2}{1+p^2}, \quad s = \frac{t(1-t)z(p)}{1-tz(p)} .$$

Vacuum polarization

$$\overline{Q}_3(b) = \int_0^\infty dp \left\{ -\frac{1}{2}\left[\sqrt{1+(bp)^2} - 1 - \frac{(bp)^2}{2}\right] \frac{1 - p\arctan\left(\frac{1}{p}\right)}{p^2} \times \right.$$

$$\times \int_0^1 \frac{dt}{t(1-t)} \frac{s(1+s)\ln(s)}{1-s} + \left[\frac{[1+(bp)^2]^{3/2}}{b^2} - \frac{1}{b^2} - \frac{3}{2}p^2 - \frac{3}{8}b^2p^4\right] \times$$

$$\times \left[-\frac{\left[2\arctan\left(\frac{1}{p}\right)\right]^3 - 2\arctan\left(\frac{1}{p}\right)\left[\pi^2 - 6\,\mathrm{dilog}\left(\frac{1}{p^2+1}\right)\right]}{12p} - \right.$$

$$\left. -\frac{\frac{1}{3} + 2\ln(p)}{p^4}\right] + \left[\sqrt{1+(bp)^2} - 1 - \frac{(bp)^2}{2} - \right.$$

$$\left. \left. -\mathrm{arctanh}\left(\frac{1}{\sqrt{1+(bp)^2}}\right) - \ln\left(\frac{pb}{2}\right) + \frac{(pb)^2}{4}\right] \times \right.$$

Vacuum polarization

$$\times\left[\frac{\left[2\arctan\left(\frac{1}{p}\right)\right]^2}{2}-\frac{\pi^2-6\,\mathrm{dilog}\left(\frac{1}{p^2+1}\right)}{6}-\frac{1-2\ln(p)}{p^2}\right]+$$

$$+\left[\frac{1}{\sqrt{1+(bp)^2}}-1+\frac{(bp)^2}{2}\right]\times$$

$$\times\left[-\frac{\int_0^1\frac{dt}{t(1-t)}(1-s)\left[\ln(1-s)\ln(s)+\mathrm{dilog}(1-s)\right]}{4p^2}+\frac{\zeta(3)}{p^2}\right]+$$

$$+\left[\mathrm{arctanh}\left(\frac{1}{\sqrt{1+(bp)^2}}\right)+\ln\left(\frac{pb}{2}\right)-\frac{(pb)^2}{4}\right]\times$$

$$\times\left[\frac{\left[2\arctan\left(\frac{1}{p}\right)\right]^2\ln(1+p^2)-\int_0^1\frac{dt}{t(1-t)}s\ln^2\left(\frac{1-t}{t[1-tz(p)]}\right)}{4p^2}+\frac{\zeta(3)}{p^2}\right]\Bigg\}.$$

Vacuum polarization

- The ultraviolet divergences are proportional to linear term in b.
- The whole expression diverges at $b = 0$.
- If everything up to linear term in b is removed then for
  - ordinary hydrogen we get precisely the result of Wichmann and Kroll
  - muonic hydrogen we get
    $(\Delta E)_{\mathrm{WK}}(2\mathrm{p}) - (\Delta E)_{\mathrm{WK}}(2\mathrm{s}) \simeq -0.10158\,10^{-5}\mathrm{eV}$
    J. Zamastil, D. Šimsa, Ann. Phys. **379**, 131 (2017)
    which differs by 1% from the result $-0.103\,10^{-5}\mathrm{eV}$
    E. Borie, Ann. Phys. (NY) **327**, 733 (2012)
    S. G. Karshenboim et al, Phys. Rev. A **81**, 060501(R) (2010).
- According to the standard view the charge can be renormalized at any value of momentum transfer b
- Here, it has to be renormalized at zero momentum transfer $b = 0$.

Conlusions

The radius proton puzzle is not influenced by the uncertainity of the one-loop QED corrections.

Acknowledgement

Thanks to

- To Vojtěch Patkóš and Dan Šimsa for collaboration
- To you for your attention