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# Quantum electrodynamics of atomic and molecular systems

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# Introduction

Quantum electrodynamics theory

- gives almost complete description of atomic systems,
- accounts for the electron self-energy and the vacuum polarization,
- goes beyond instantaneous Coulomb interaction between electrons,
- and suplemented by the Standard Model gives description of the interaction at high energies

# Contents

**I** Theory of Lamb shift in hydrogenic sysems:

H, $He^+$, $\mu$H, $\mu^+ e^-$, $e^+ e^-$

**II** QED of few electron atomic systems:

He, Li and $H_2$

# Proton charge radius puzzle

- finite nuclear size effect

$$\Delta E = E_{\rm exp} - E_{\rm the} = \frac{2}{3\,n^3}\,(Z\,\alpha)^4\,\mu^3\,\langle r_p^2\rangle$$

- global fit to H and D spectrum: $r_p = 0.8758(77)$ fm (CODATA 2010)
- $e - p$ scattering: $r_p = 0.886(8)$ (Sick, 2012)
- from muonic hydrogen: $r_p = 0.84184(67)$ fm (PSI, 2010)

If all measurements are correct, this discrepancy does not find any explanation within the known description of electromagnetic, weak and strong interactions.

# Theory of hydrogenic energy levels

- From the Dirac equation the ground state energy of an electron in the Coulomb field is

$$E = m\sqrt{1-\alpha^2},$$

where $\hbar = c = 1$ for convenience.

- The Taylor series of $E$ is

$$E = m\left[1 - \frac{\alpha^2}{2} - \frac{\alpha^4}{8} - \frac{\alpha^6}{16} + O(\alpha^8)\right]$$

- The first term is the rest mass $m$ or equivalently the rest energy.
- The second term is the nonrelativistic binding energy, in agreement to the Schrödinger equation.

# Theory of hydrogenic energy levels

$$E = m\left[1 - \frac{\alpha^2}{2} - \frac{\alpha^4}{8} - \frac{\alpha^6}{16} + O(\alpha^8)\right]$$

- The third term is the leading relativistic correction, which can be expressed as the expectation value of

$$-\frac{\alpha^4}{8} = \left\langle \phi \left| -\frac{p^4}{8\,m^3} + \frac{\pi\,\alpha}{2}\delta^{(3)}(r) \right| \phi \right\rangle$$

  with the ground state nonrelativistic wave function $\phi$.
- The fourth term, proportional to $\alpha^6$, is the higher order relativistic correction. It can be expressed as the combination of expectation values with nonrelativistic wave function, but it is little more complicated, as individual matrix elements are singular.
- The leading QED effects are of order $\alpha^5$, more precisely $\alpha\,(Z\,\alpha)^4$, where $Z\,e$ is a charge of the nucleus

# Theory of hydrogen energy levels

- energy according to Dirac equation

$$f(n,j) = \left(1 + \frac{(Z\,\alpha)^2}{[n+\sqrt{(j+1/2)^2-(Z\,\alpha)^2}-j-1/2]^2}\right)^{-1/2}$$

- total energy

$$\begin{aligned} E &= M + m + \mu[f(n,j)-1] - \frac{\mu^2}{2\,M}[f(n,j)-1]^2 \\ &\quad + \frac{(Z\,\alpha)^4\,\mu^3}{2\,n^3\,M}\left[\frac{1}{j+1/2} - \frac{1}{l+1/2}\right](1-\delta_{l0}) + E_L \end{aligned}$$

- $E_L(\alpha) = E^{(5)} + E^{(6)} + E^{(7)} + E^{(8)} + \ldots$ where $E^{(n)} \sim \alpha^n\,\mathcal{E}^{(n)}$

# Green function versus binding energy

The energy level can be interpreted as a pole of $G(E)$ as a function of $E$.

$$\langle\phi|G(E)|\phi\rangle = \langle\phi|\frac{1}{E - H_0 - \Sigma(E)}|\phi\rangle \equiv \frac{1}{E - E_0 - \sigma(E)},$$

where

$$\sigma(E) = \langle\phi|\Sigma(E)|\phi\rangle + \sum_{n\neq 0}\langle\phi|\Sigma(E)|\phi_n\rangle\,\frac{1}{E - E_n}\,\langle\phi_n|\Sigma(E)|\phi\rangle + \dots$$

Having $\sigma(E)$, the correction to the energy level can be expressed as

$$\begin{aligned}
\delta E &= E - E_0 = \sigma(E_0) + \sigma'(E_0)\,\sigma(E_0) + \dots \\
&= \langle\phi|\Sigma(E_0)|\phi\rangle + \langle\phi|\Sigma(E_0)\,\frac{1}{(E_0 - H_0)'}\,\Sigma(E_0)|\phi\rangle \\
&\quad + \langle\phi|\Sigma'(E_0)|\phi\rangle\,\langle\phi|\Sigma(E_0)|\phi\rangle + \dots \\
\Sigma(E_0) &= H^{(4)} + H^{(5)} + H^{(6)} + \dots
\end{aligned}$$

# Contributions to the Lamb shift

- one-loop electron self-energy and vacuum polarization
- two-loops
- three-loops
- pure recoil correction
- radiative recoil correction
- finite nuclear size, and polarizability

# One-loop contribution

$$\delta_{SE}E = \frac{e^2}{(2\pi)^4 i}\int d^d k \frac{1}{k^2}\langle\bar{\psi}|\gamma^\mu \frac{1}{\not{p}-\not{k}+\gamma^0 Z\alpha/r - m}\gamma_\mu|\psi\rangle - \delta m\langle\bar{\psi}|\psi\rangle$$

$$\delta_{VP}E = \langle\bar{\psi}|\gamma^0 U_{VP}|\psi\rangle$$

$$U_{VP}(\vec{r}) = -\alpha\int d^3r' \frac{\rho_{VP}(\vec{r}')}{|\vec{r}-\vec{r}'|}$$

$$\rho_{VP}(\vec{r}') = i\int_{-\infty}^{\infty}\frac{dz}{2\pi}\sum_n \frac{\psi_n^+(\vec{r}')\,\psi_n(\vec{r}')}{z - E_n(1-i\epsilon)}$$

# One-loop contribution

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

analytic expansion

$$F(Z\alpha) = A_{40} + A_{41}\,\ln(Z\alpha)^{-2} + (Z\alpha)\,A_{50}$$
$$+(Z\alpha)^2\,[A_{62}\,\ln^2(Z\alpha)^{-2} + A_{61}\,\ln(Z\alpha)^{-2} + A_{60} + O(Z\alpha)]$$

or direct numerical evaluation using
the exact Coulomb-Dirac propagator

# NRQED: Example calculation of leading terms

NRQED Hamiltonian

$$
\begin{aligned}
H_{\mathrm{NRQED}} &= \frac{\vec{\pi}^2}{2\,m} + e\,A^0 - \frac{e}{6}\left(\frac{3}{4\,m^2} + r_E^2\right)\vec{\nabla}\cdot\vec{E} - \frac{\vec{\pi}^4}{8\,m^3} \\
&\quad - \frac{e}{2\,m}\,g\,\vec{s}\cdot\vec{B} - \frac{e}{4\,m^2}\,(g-1)\,\vec{s}\cdot\left(\vec{E}\times\vec{\pi} - \vec{\pi}\times\vec{E}\right)
\end{aligned}
$$

where $\vec{\pi} = \vec{p} - e\,\vec{A}$, $g = 2\,(1+\kappa)$, $\kappa = \alpha/(2\,\pi)$ and

$$
r_E^2 = \frac{3\,\kappa}{2\,m^2} + \frac{2\,\alpha}{\pi\,m^2}\left(\ln\frac{m}{2\,\epsilon} + \frac{11}{24}\right)
$$

Without QED: $r_E^2 = \kappa = 0$, and the effective Hamiltonian $H_{\mathrm{NRQED}}$ is the nonrelativistic approximation to the Dirac Hamiltonian. At this form it includes “hard” radiative effects.

# NRQED: Lamb shift in the hydrogen atom

The leading QED correction to hydrogenic energy levels is obtained from the above Hamiltonian by splitting it into the low and high energy parts

$$\delta E = \delta E_L + \delta E_H \,.$$

The high energy part is the expectation value of $r_E^2\,\vec{\nabla}\cdot\vec{E}$ term in the NRQED Hamiltonian

$$\delta E_H = \left\langle -\frac{e}{6}\, r_E^2\, \vec{\nabla}\cdot\vec{E} \right\rangle = \frac{2}{3}\,\frac{(Z\,\alpha)^4}{n^3}\, r_E^2\,\delta_{l0} = \frac{\alpha}{\pi}\,\frac{(Z\,\alpha)^4}{n^3}\left(\frac{4}{3}\,\ln\frac{m}{2\,\epsilon}+\frac{10}{9}\right)\delta_{l0},$$

# NRQED: Lamb shift in the hydrogen atom

while the low energy part is due to emission and absorption of the low energy ($k < \epsilon$) photon

$$\begin{aligned}\delta E_L &= e^2 \int_0^{\epsilon} \frac{d^3 k}{(2\pi)^3\, 2k} \left(\delta^{ij} - \frac{k^i k^j}{k^2}\right) \left\langle \frac{p^i}{m} \frac{1}{E-H-k} \frac{p^j}{m} \right\rangle \\ &= \frac{2\alpha}{3\pi} \left\langle \frac{\vec{p}}{m} (H-E) \left\{ \ln\left[\frac{2\epsilon}{m(Z\alpha)^2}\right] - \ln\left[\frac{2(H-E)}{m(Z\alpha)^2}\right] \right\} \frac{\vec{p}}{m} \right\rangle\end{aligned}$$

where $\vec{E} = -\vec{\nabla} A^0$, $A^0 = -Z e/(4\pi r)$. The vacuum polarization can be accounted for by adding to $r_E^2$ a term $-2\alpha/(5\pi m^2)$, so the total Lamb shift becomes

$$\delta E = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n^3} \left\{ \frac{4}{3} \ln\left[(Z\alpha)^{-2}\right] \delta_{l0} + \left(\frac{10}{9} - \frac{4}{15}\right) \delta_{l0} - \frac{4}{3} \ln k_0(n,l) \right\}$$

where

$$\ln k_0(n,l) = \frac{n^3}{2 m^3 (Z\alpha)^4} \left\langle \vec{p}\,(H-E) \ln\left[\frac{2(H-E)}{m(Z\alpha)^2}\right] \vec{p} \right\rangle$$

and $\ln\epsilon$ terms cancels out, as expected.

# NRQED: Lamb shift in the hydrogen atom

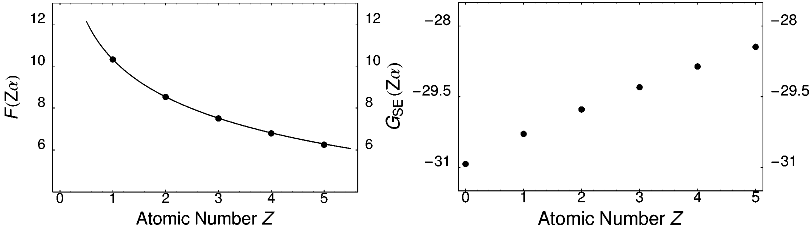
General one loop result: [Phys. Rev. Lett. **95**, 180404 (2005)]

$$
\begin{aligned}
\delta^{(1)}E \;=\;& \frac{\alpha}{\pi}\,\frac{(Z\,\alpha)^4}{n^3}\left\{\left[\frac{10}{9}+\frac{4}{3}\,\ln\left[(Z\,\alpha)^{-2}\right]\right]\delta_{l0}-\frac{4}{3}\,\ln k_0\right\}+\frac{Z\,\alpha^2}{4\,\pi}\left\langle\sigma^{ij}\nabla^i V p^j\right\rangle \\
&+\frac{\alpha}{\pi}\left\{\frac{(Z\,\alpha)^6}{n^3}\,\mathcal{L}+\left(\frac{5}{9}+\frac{2}{3}\,\ln\left[\tfrac{1}{2}\,(Z\,\alpha)^{-2}\right]\right)\left\langle\vec{\nabla}^2 V\,\frac{1}{(E-H)'}\,H_R\right\rangle\right. \\
&+\frac{1}{2}\left\langle\sigma^{ij}\nabla^i V p^j\,\frac{1}{(E-H)'}\,H_R\right\rangle+\left(\frac{779}{14400}+\frac{11}{120}\,\ln\left[\tfrac{1}{2}\,(Z\,\alpha)^{-2}\right]\right)\langle\vec{\nabla}^4 V\rangle \\
&+\left(\frac{23}{576}+\frac{1}{24}\,\ln\left[\tfrac{1}{2}\,(Z\,\alpha)^{2}\right]\right)\langle 2\,\mathrm{i}\,\sigma^{ij}\,p^i\vec{\nabla}^2 V p^j\rangle+\frac{3}{80}\,\langle\vec{p}^{\,2}\,\vec{\nabla}^2 V\rangle \\
&\left.+\left(\frac{589}{720}+\frac{2}{3}\,\ln\left[\tfrac{1}{2}\,(Z\,\alpha)^{2}\right]\right)\langle(\vec{\nabla}V)^2\rangle-\frac{1}{8}\,\langle\vec{p}^{\,2}\,\sigma^{ij}\,\nabla^i V p^j\rangle\right\} \\
&+\alpha^3\,X\left\langle\vec{\nabla}^2 V\right\rangle .
\end{aligned}
$$

# Numerical evaluation of the one-loop self-energy

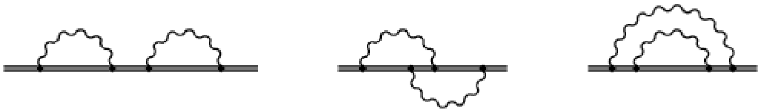
[U. Jentschura, P.J. Mohr, and G. Soff, Phys. Rev. Lett. **82**, 53 (1999)]

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




$$\begin{aligned} F(Z\alpha) &= A_{40} + A_{41} \ln(Z\alpha)^{-2} + (Z\alpha) A_{50} \\ &\quad + (Z\alpha)^2 \left[A_{62} \ln^2(Z\alpha)^{-2} + A_{61} \ln(Z\alpha)^{-2} + G_{60}\right] \end{aligned}$$

# Two-loop electron self-energy correction

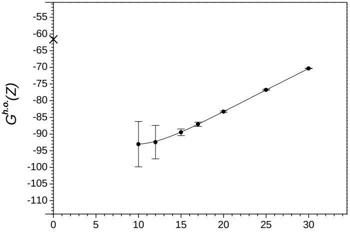


Electron propagators include external Coulomb field, external legs are bound state wave functions.

The expansion of the energy shift in powers of $Z\alpha$

$$
\begin{aligned}
\delta^{(2)}E &= m\left(\frac{\alpha}{\pi}\right)^2 F(Z\alpha) \\
F(Z\alpha) &= B_{40} + (Z\alpha)\,B_{50} + (Z\alpha)^2\left\{[\ln(Z\alpha)^{-2}]^3\,B_{63}\right. \\
&\quad \left. +[\ln(Z\alpha)^{-2}]^2\,B_{62} + \ln(Z\alpha)^{-2}\,B_{61} + G(Z\alpha)\right\}
\end{aligned}
$$

# Direct numerical calculation versus analytical expansion




$G_{60}(1) \approx -86(15)$ $(\mathrm{Yerokhin}, 2009)$, uncertainty $\delta E(1S) = \pm 1.5$ kHz

$B_{60} = -61.6(9.2)$ $(\mathrm{K.P., U.J.}, 2003)$

uncertainty due to the unknown high energy contribution from the class of about 80 diagrams

discrepancy in the proton charge radius $\to \delta E(1S) \approx 100$ kHz

# Pure recoil corrections

- finite nuclear mass effects, beyond the Dirac equation
- leading $O(\alpha^5)$ terms are known for an arbitrary mass ratio

$$
\begin{aligned}
\delta E^{(5)} \quad = \quad & \frac{\mu^3}{m\,M}\,\frac{(Z\,\alpha)^5}{\pi\,n^3}\left\{\frac{1}{3}\,\delta_{l0}\,\ln(Z\,\alpha)^{-2}-\frac{8}{3}\,\ln k_0(n,l)-\frac{1}{9}\,\delta_{l0}-\frac{7}{3}\,a_n\right. \\
& \left.-\frac{2}{M^2-m^2}\,\delta_{l0}\left[M^2\,\ln\frac{m}{\mu}-m^2\,\ln\frac{M}{\mu}\right]\right\}
\end{aligned}
$$

where

$$
a_n=-2\left[\ln\frac{2}{n}+\left(1+\frac{1}{2}+\cdots+\frac{1}{n}\right)+1-\frac{1}{2\,n}\right]\delta_{l0}+\frac{1-\delta_{l0}}{l\,(l+1)\,(2\,l+1)}
$$

# Pure recoil corrections

- higher order terms from the exact in $Z\,\alpha$ formula for the leading correction in the mass ratio $O(m/M)$

$$\delta E = \frac{i}{2\,\pi\,M}\int_{-\infty}^{\infty} d\omega\, \langle\psi|\left[\vec{p}-\vec{D}(\omega)\right]\, G(E+\omega)\,\left[\vec{p}-\vec{D}(\omega)\right]|\psi\rangle$$

where

$$G(E) = \frac{1}{E-H_D}$$
$$D^j(\omega) = -4\,\pi\,Z\,\alpha\,D^{jk}(\omega)\,\alpha^k$$
$$D^{jk}(\omega,\vec{r}) = -\frac{1}{4\,\pi}\left[\frac{e^{i\,|\omega|\,r}}{r}\,\delta^{jk} + \nabla^j\nabla^k\,\frac{e^{i\,|\omega|\,r}-1}{\omega^2\,r}\right]$$

$D$ is a photon propagator in a Coulomb gauge

# Radiative recoil corrections

- accomodated in the $Z\,\alpha$ expansion coefficient of the electron self-energy and the vacuum-polarization

$$
\begin{aligned}
\delta E &= \frac{m\,\alpha\,(Z\,\alpha)^4}{\pi\,n^3}\left(\frac{\mu}{m}\right)^3 F(Z\,\alpha) \\
F(Z\,\alpha) &= A_{40} + A_{41}\,\ln[(Z\,\alpha)^{-2}\,m/\mu] + (Z\,\alpha)\,A_{50} \\
&+(Z\,\alpha)^2\,\{A_{62}\,\ln^2[(Z\,\alpha)^{-2}\,m/\mu] + A_{61}\,\ln[(Z\,\alpha)^{-2}\,m/\mu] + A_{60} + O(Z\,\alpha)\}
\end{aligned}
$$

$$
A_{40}(n,l\neq 0) = \frac{m}{\mu}\,\frac{2\,(j-l)\,(j+1/2)}{2\,(2\,l+1)} - \frac{4}{3}\,\ln k_0(n,l)
$$

- the remainder

$$
\delta E^{(6)} = \frac{\mu^3}{m\,M}\,\frac{\alpha\,(Z\,\alpha)^5}{\pi^2\,n^3}\,\delta_{l0}\left[6\,\zeta(3) - 2\,\pi^2\,\ln 2 + \frac{35\,\pi^2}{36} - \frac{448}{27}\right]
$$

# Nuclear size and polarizability corrections

- nuclear self-energy: corrections to formfactors are infrared divergent

$$\delta E = \frac{4\,Z^2\,\alpha\,(Z\,\alpha)^4}{3\,\pi\,n^3}\,\frac{\mu^3}{M^2}\left[\ln\left(\frac{M}{\mu\,(Z\,\alpha)^2}\right)\delta_{l0} - \ln\,k_0(n,l)\right]$$

- higher order finite size

$$E_{FS} = \mathcal{E}_{FS}\left\{1 - C_\eta\,\frac{r_p}{\lambda\!\!\!^-}\,Z\,\alpha - \left[\ln\left(\frac{r_p\,Z\,\alpha}{\lambda\!\!\!^-\,n}\right) + \psi(n) + \gamma - \frac{(5\,n+9)\,(n-1)}{4\,n^2} - C_\theta\right](Z\,\alpha)^2\right\}$$

where $C_\eta = 1.7(1)$ and $C_\theta = 0.47(4)$

- finite size combined with SE and VP $\sim O(Z\,\alpha^2)$
- proton polarizability: $\delta_{\rm pol}E = -0.087(16)\,\frac{\delta_{l0}}{n^3}\,h\,kHz$

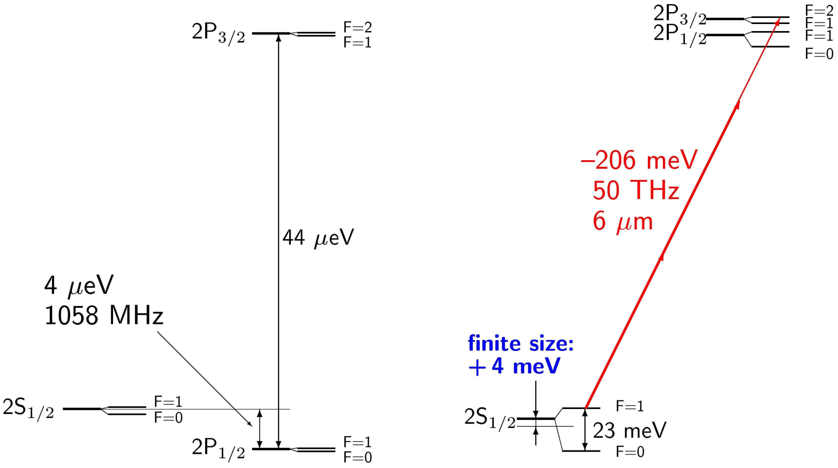
# Experimental results for hydrogen and $r_p$

Some more accurate results

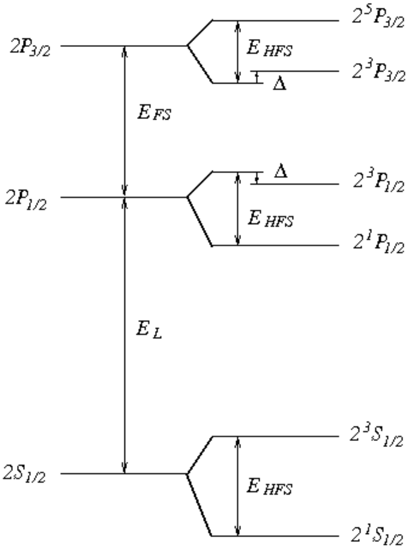
- $\nu_{exp.}(2P_{1/2} - 2S_{1/2}) = 1\,057\,845.0(9.0)$ kHz, [Lundeen, Pipkin, 1994]
- $\nu_{\mathrm{exp}}(1S_{1/2} - 2S_{1/2}) = 2\,466\,061\,413\,187.035(10)$ kHz, [MPQ, 2011]
- $\nu_{\mathrm{exp}}(2S_{1/2} - 8D_{5/2}) = 770\,859\,252\,849.5(5.9)$ kHz, [Paris, 2001]
- global fit to the hydrogen data $\Rightarrow$

$$r_p = 0.875\,8(77)\ \mathrm{fm}$$

# energy levels of $\mu$H in comparison to H



# energy levels of $\mu$H




$E_L = 202.1\ meV$

$E_{FS} = 8.4\ meV$

$E_{HFS}(2S_{1/2}) = 22.7\ meV$

$E_{HFS}(2P_{1/2}) = 8.0\ meV$

$E_{HFS}(2P_{3/2}) = 3.4\ meV$

$\Delta = 0.1\ meV$

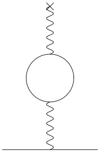
# Theory of $\mu H$ energy levels

- $\mu H$ is essentially a nonrelativistic atomic system
- muon and proton are treated on the same footing
- $m_\mu / m_e = 206.768 \Rightarrow \beta = m_e/(\mu\,\alpha) = 0.737$ the ratio of the Bohr radius to the electron Compton wavelength
- the electron vacuum polarization dominates the Lamb shift

$$E_L = \int d^3 r\, V_{vp}(r)\,(\rho_{2P} - \rho_{2S}) = 205.006\,\mathrm{meV}$$

- important corrections: second order, two-loop vacuum polarization, and the muon self-energy
- other corrections are much smaller than the discrepancy of 0.3 meV.

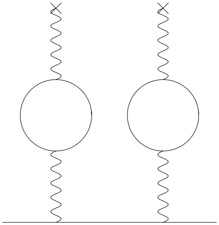
# One-loop electron vacuum-polarization



- the electron loop modifies the Coulomb interaction by

$$
\begin{aligned}
V_{vp}(r) &= -\frac{Z\,\alpha}{r}\,\frac{\alpha}{\pi}\int_4^\infty \frac{d(q^2)}{q^2}\,e^{-m_e\,q\,r}\,u(q^2)\\
u(q^2) &= \frac{1}{3}\sqrt{1-\frac{4}{q^2}}\left(1+\frac{2}{q^2}\right)\\
E_L &= \langle 2P|\,V_{vp}|2P\rangle - \langle 2S|\,V_{vp}|2S\rangle\\
R_{2S} &= \frac{1}{\sqrt{2}}\,e^{-\frac{\mu\,\alpha\,r}{2}}\left(1-\frac{\mu\,\alpha\,r}{2}\right),\quad R_{2P} = \frac{1}{2\,\sqrt{6}}\,e^{-\frac{\mu\,\alpha\,r}{2}}\,(\mu\,\alpha\,r)
\end{aligned}
$$

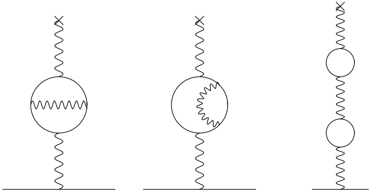
# Double vp correction



$$
\begin{aligned}
E_L &= \langle\phi| V_{vp} \frac{1}{(E-H)'} V_{vp}|\phi\rangle \\
&= \mu\,(Z\,\alpha)^2 \left(\frac{\alpha}{\pi}\right)^2 \frac{4}{9}\, 0.0124 \\
&= 0.151\,\mathrm{meV}\,.
\end{aligned}
$$

finite nuclear mass included in the reduced mass treatment

# Two-loop vacuum polarization



$$E_L = \int \frac{d^3p}{(2\,\pi)^3}\,\rho(p)\,\frac{4\,\pi\,\alpha}{p^2}\,\bar{\omega}^{(2)}(-p^2)$$

$$= \mu\,(Z\,\alpha)^2\,\left(\frac{\alpha}{\pi}\right)^2\,0.0552667 = 1.508\,\mathrm{meV}$$

# Leading relativistic correction

$$
\begin{aligned}
\delta H &= -\frac{p^4}{8\,m^3} - \frac{p^4}{8\,M^3} + \frac{\alpha}{r^3}\left(\frac{1}{4\,m^2} + \frac{1}{2\,m\,M}\right)\vec{r}\times\vec{p}\cdot\vec{\sigma} \\
&\quad + \frac{\pi\,\alpha}{2}\left(\frac{1}{m^2} + \frac{1}{M^2}\right)\delta^3(r) - \frac{\alpha}{2\,m\,M\,r}\left(p^2 + \frac{\vec{r}\,(\vec{r}\vec{p})\,\vec{p}}{r^2}\right)
\end{aligned}
$$

$$
\begin{aligned}
\delta E &= \langle l, j, m_j | \delta H | l, j, m_j \rangle \\
&= \frac{(Z\,\alpha)^4\,\mu^3}{2\,n^3\,m_p^2}\left(\frac{1}{j+\frac{1}{2}} - \frac{1}{l+\frac{1}{2}}\right)(1-\delta_{l0})
\end{aligned}
$$

$$
\delta E_L = \frac{\alpha^4\mu^3}{48\,m_p^2} = 0.057\mathrm{meV}
$$

valid for an arbitrary mass ratio

# Relativistic correction to the one-loop vp

assume that photon has a mass $\rho$

$$
\begin{aligned}
V_{vp} &= -\frac{\alpha}{r}\, e^{-\rho\, r} \\
\delta H_{vp} &= \frac{\alpha}{8}\left(\frac{1}{m^2}+\frac{1}{M^2}\right)\left(4\,\pi\,\delta^3(r)-\frac{\rho^2}{r}\,e^{-\rho\, r}\right)-\frac{\alpha\,\rho^2}{4\,m\,M}\,\frac{e^{-\rho r}}{r}\left(1-\frac{\rho\, r}{2}\right) \\
&\quad -\frac{\alpha}{2\,m\,M}\,p^i\,\frac{e^{-\rho r}}{r}\left(\delta_{ij}+\frac{r_i\, r_j}{r^2}\,(1+\rho\, r)\right)p^j \\
&\quad +\frac{\alpha}{r^3}\left(\frac{1}{4\,m^2}+\frac{1}{2\,m\,M}\right)e^{-\rho\, r}\,(1+\rho\, r)\,\vec{r}\times\vec{p}\cdot\vec{\sigma}\,.
\end{aligned}
$$

The relativistic correction to the energy due to the exchange of the massive photon is given by

$$
E(\rho)=\langle\phi|\delta H_{vp}|\phi\rangle+2\,\langle\phi|(\delta H+\delta V)\,\frac{1}{(E-H)'}\,V_{vp}|\phi\rangle \text{ with } H=\frac{p^2}{2\,\mu}-\frac{\alpha}{r}
$$

$$
\delta E_L=\frac{\alpha}{\pi}\int_4^\infty \frac{d(\rho^2)}{\rho^2}\,u\left(\frac{\rho^2}{m^2}\right)\left(E_{2P_{1/2}}(\rho)-E_{2S_{1/2}}(\rho)\right)=0.0188\,\mathrm{meV}\,.
$$

[Jentschura 2011, Karshenboim 2012]

# Muon self-energy and muon vp

$$
\begin{aligned}
E(2S_{1/2}) &= \frac{1}{8}\, m_\mu \,\frac{\alpha}{\pi}\,(Z\,\alpha)^4 \left(\frac{\mu}{m_\mu}\right)^3 \left\{\frac{10}{9} - \frac{4}{15} - \frac{4}{3}\ln k_0(2S)\right. \\
&\quad \left. + \frac{4}{3}\ln\left(\frac{m_\mu}{\mu\,(Z\,\alpha)^2}\right) + 4\,\pi\,Z\,\alpha\left(\frac{139}{128} + \frac{5}{192} - \frac{\ln(2)}{2}\right)\right\} \\
E(2P_{1/2}) &= \frac{1}{8}\, m_\mu \,\frac{\alpha}{\pi}\,(Z\,\alpha)^4 \left(\frac{\mu}{m_\mu}\right)^3 \left\{-\frac{1}{6}\,\frac{m_\mu}{\mu} - \frac{4}{3}\ln k_0(2P)\right\} \\
E_L &= -0.668\,\mathrm{meV}\,.
\end{aligned}
$$

# $O(\alpha^5)$ recoil correction

- pure recoil coorection

$$
\begin{aligned}
E(n,l) &= \frac{\mu^3}{m_\mu\, m_p}\frac{(Z\,\alpha)^5}{\pi\, n^3}\left\{\frac{2}{3}\,\delta_{l0}\,\ln\left(\frac{1}{Z\,\alpha}\right)-\frac{8}{3}\,\ln k_0(n,l)-\frac{1}{9}\,\delta_{l0}-\frac{7}{3}\,a_n\right. \\
&\left.-\frac{2}{m_p^2-m_\mu^2}\,\delta_{l0}\left[m_p^2\,\ln\left(\frac{m_\mu}{\mu}\right)-m_\mu^2\,\ln\left(\frac{m_p}{\mu}\right)\right]\right\} \\
a_n &= -2\left(\ln\frac{2}{n}+(1+\frac{1}{2}+\ldots+\frac{1}{n})+1-\frac{1}{2\,n}\right)\delta_{l0}+\frac{1-\delta_{l0}}{l\,(l+1)\,(2\,l+1)}
\end{aligned}
$$

It contributes the amount of

$$
\delta E_L = -0.045\,\mathrm{meV}\,.
$$

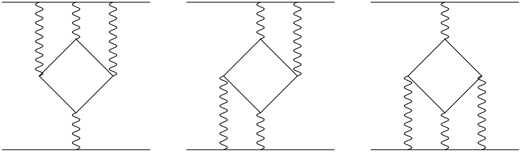
- proton self-energy

$$
E(n,l) = \frac{4\,\mu^3\,(Z^2\,\alpha)\,(Z\,\alpha)^4}{3\,\pi\,n^3\,m_p^2}\left(\delta_{l0}\,\ln\left(\frac{m_p}{\mu\,(Z\,\alpha)^2}\right)-\ln k_0(n,l)\right)\,. \qquad (1)
$$

It contributes

$$
\delta E_L = -0.010\,\mathrm{meV}\,. \qquad (2)
$$

# Light by light diagrams



- $\delta E_L = -0.0009$ meV
- significant cancellation between diagrams
- S.G. Karshenboim *et al.*, arXiv:1005.4880

# Proton finite size correction

- in muonic atoms nuclear finite size effects give a large contribution to energy levels:

$$E_{FS} = \frac{2\,\pi\,\alpha}{3}\,\phi^2(0)\,\langle r_p^2\rangle\,\delta_{l0}$$

$$\phi^2(0) = \frac{(\mu\,\alpha)^3}{\pi}\,\delta_{l0}$$

- relativistic corrections to $\phi^2(0)$
- electron vp corrections to $\phi^2(0)$
- muon self-energy correction to $\phi^2(0)$
- in total: $E_{FS} = -5.2262\, r_p^2/\mathrm{fm}^2$ meV

# Definition of the nuclear charge radius

- $G_E(-\vec{Q}^2) = 1 - \frac{\langle r^2 \rangle}{6}\, \vec{Q}^2 + O(q^4)$
- Low energy interaction Hamiltonian with the electromagnetic field

$$\delta H = e\, A^0 - e \left( \frac{\langle R^2 \rangle}{6} + \frac{\delta_I}{M^2} \right) \vec{\nabla} \cdot \vec{E} - \frac{e}{2}\, Q\, (I^i\, I^j)^{(2)}\, \nabla^j E^i - \vec{\mu} \cdot \vec{B}$$

- $\mu$ and $Q$ are the magnetic dipole and the electric quadrupole moments, respectively
- for a scalar particle $\delta_0 = 0$
- for a half-spin particle $\delta_{1/2} = 1/8$
- for a spin 1 particle $\delta_0 = 0$, but it is somewhat arbitrary
- $E_{FS} = \frac{2\,\pi\,\alpha}{3}\, \phi^2(0)\, \langle R^2 \rangle = -3.9$ meV for $2P - 2S$ transition
- nuclear structure corrections ?

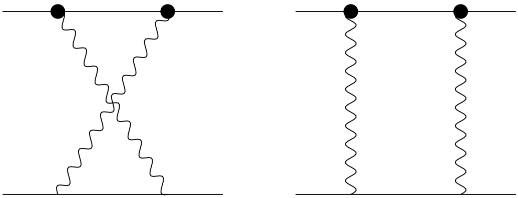
# Further small corrections

- fine and hyperfine structure from the Breit-Pauli Hamiltonian
- three-loop electronic vp
- muon self-energy combined with the electronic vp (on a Coulomb and self-energy photon)
- higher order $O(\alpha^6)$ recoil corrections
- proton structure: elastic and inelastic corrections
- hadronic vp

# Nuclear structure effects

- when nuclear excitation energy is much larger than the atomic energy, the two-photon exchange scattering amplitude gives the dominating correction

- the total proton structure contribution $\delta E_L = 36.9(2.4)\ \mu\text{eV}$ is much too small to explain the discrepancy



# Final results

- $\Delta E = E(2P_{3/2}(F=2)) - E(2S_{1/2}(F=1))$
- experimental result: $\Delta E = 206.2949(32)$ meV
- total theoretical result from [U. Jenschura, 2011]

$$\Delta E = \left(209.9974(48) - 5.2262\frac{r_p^2}{\mathrm{fm}^2}\right)\,\mathrm{meV} \;\Rightarrow$$

- $r_p = 0.841\,69(66)$ fm

# Analysis of discrepancy

possible sources of discrepancy:

- mistake in the QED calculations ? $\mu$H checked by many and only few corrections contribute at the level of discrepancy
- vp verified by an agreement $\sim 10^{-6}$ for $3D - 2P$ transition in $^{24}$Mg and $^{28}$Si
- large Zemach moment $(r_p^{(2)})^3$ ruled out by the low energy electron-proton scattering [Friar, Sick, 2005], [Cloët, Miller, 2010], [Distler, Bernauer, Walcher, 2010]
- nuclear polarizability correction ? much too small
- possible new light particles ? ruled out by muon $g - 2$ and other low energy Standard Model tests: Barger *et al.*, Phys. Rev. Lett. **106**, 153001 (2011), **108**, 081802 (2012)
- violation of the universality in the lepton-proton interaction ? [Camilleri, *et al*, 1969]
- wrong Rydberg constant, [Randolf Pohl, 2010]