Isotope shifts with highly charged ions

Vladimir M. Shabaev

St. Petersburg State University

Russia

Outline of the talk

- Introduction
- Isotope shifts of the binding energies
  - Nuclear recoil
  - Nuclear size
  - Nuclear polarization
- Isotope shifts of the g factors
- Conclusion

Introduction

The isotope shift of the binding energy is basically given by a sum of the mass and field shifts:

$$\delta E = \delta E^{(\mathrm{MS})} + \delta E^{(\mathrm{FS})} \,.$$

The mass shift is due to the nuclear recoil effect. In the nonrelativistic theory this effect is determined by the operator *(D.S. Hughes and C. Eckart, Phys. Rev., 1930):*

$$H_M = \frac{1}{2M} \sum_i \vec{p}_i^{\,2} + \frac{1}{2M} \sum_{i \neq j} (\vec{p}_i \cdot \vec{p}_j) \,.$$

Here the first and second terms define so-called normal and specific mass shifts. To the first order in the electron-to-nucleus mass ratio, the mass shift can be evaluated as

$$\delta E^{(\mathrm{MS})} = \langle \Psi | (H_{M_1} - H_{M_2}) | \Psi \rangle \,.$$

Introduction

The field shift is due to the nuclear size effect. This effect is mainly determined by the rms nuclear charge radius $R = \langle r^2 \rangle^{1/2}$. The energy difference between two isotopes can be approximated as

$$\delta E^{(\mathrm{FS})} = F \delta \langle r^2 \rangle \, ,$$

where F is the field-shift factor and $\delta \langle r^2 \rangle$ is the mean-square charge radius difference. In accordance with this definition, the F factor can be calculated by

$$F = \frac{dE(R)}{d\langle r^2 \rangle} \, .$$

Neglecting the variation of the electronic density inside the nucleus yields

$$F = \frac{2\pi}{3} \alpha Z |\Psi(0)|^2 \, .$$

Introduction

High-precision measurements of the isotope energy shifts in B-like argon *(R. Soria Orts et al., PRL, 2006)* and in Li-like neodymium *(C. Brandau et al., PRL, 2008)* have required the fully relativistic calculations.

The experiment with Li-like Nd provided determination of the nuclear charge radius difference. The corresponding experiments can be also performed for radioactive isotopes with a lifetime longer than about 10 s *(C. Brandau et al., Hyp. Int., 2010)*.

With the FAIR facilities the measurements of the isotope energy shifts in highly charged ions will be improved in accuracy by an order of magnitude.

First measurements of the isotope shift of the g factor of highly charged ions were recently performed for Li-like calcium *(F. Köhler, K. Blaum et al., to be published)*.

From the theoretical side, to meet the required accuracy one needs to evaluate the isotope shifts including the relativistic and QED effects.

Nuclear recoil effect in the nonrelativistic theory

Nonrelativistic Hamiltonian

$$H = \frac{\vec{P}_{\rm n}^2}{2M} + \sum_i \frac{\vec{p}_i^2}{2m} - \sum_i \frac{\alpha Z}{|\vec{r}_i - \vec{R}_{\rm n}|} + \sum_{i \neq j} \frac{\alpha}{|\vec{r}_i - \vec{r}_j|}\,,$$

where $\vec{P}_{\rm n}$ is the nuclear momentum operator and $\vec{p}_i$ is the momentum operator of the i-th electron. The binding energy is determined by the Schrödinger equation:

$$H\Phi = E\Phi\,.$$

Since the total momentum of the atom conserves, $[H, \vec{P}] = 0$, we can restrict our consideration to the center-of-mass frame:

$$\vec{P}\Phi = (\vec{P}_{\rm n} + \sum_i \vec{p}_i)\Phi = 0.$$

Nuclear recoil effect in the nonrelativistic theory

Therefore, in the center-of-mass frame:

$$\vec{P}_{\rm n} = -\sum_i \vec{p}_i \,.$$

The kinetic energy of the nucleus:

$$\frac{\vec{P}_{\rm n}^2}{2M} = \frac{1}{2M}\sum_i \vec{p}_i^{\,2} + \frac{1}{2M}\sum_{i\neq j}(\vec{p}_i \cdot \vec{p}_j)\,.$$

The nonrelativistic nuclear recoil operator:

$$H_M = \frac{1}{2M}\sum_i \vec{p}_i^{\,2} + \frac{1}{2M}\sum_{i\neq j}(\vec{p}_i \cdot \vec{p}_j)\,.$$

Here the first and second terms define the so-called normal and specific mass shifts.

Nuclear recoil effect in the Breit approximation

For simplicity, we consider the nucleus as a heavy Dirac particle. Then, the Breit interaction between the nucleus and the atomic electrons:

$$V_{\rm B} = \sum_i \frac{\alpha Z}{2} \Big[\frac{(\vec{\boldsymbol{\alpha}}_{\rm n} \cdot \vec{\boldsymbol{\alpha}}_i)}{|\vec{r}_i - \vec{R}_{\rm n}|} + \frac{(\vec{\boldsymbol{\alpha}}_{\rm n} \cdot (\vec{r}_i - \vec{R}_{\rm n}))(\vec{\boldsymbol{\alpha}}_i \cdot (\vec{r}_i - \vec{R}_{\rm n}))}{|\vec{r}_i - \vec{R}_{\rm n}|^3} \Big] \,.$$

In the nonrelativistic limit for the nucleus one should replace:

$$\vec{\boldsymbol{\alpha}}_{\rm n} \to \frac{\vec{P}_{\rm n}}{M} \,.$$

We get

$$V_{\rm B} = \frac{\alpha Z}{2M} \sum_i \Big[\frac{\vec{\boldsymbol{\alpha}}_i}{|\vec{r}_i - \vec{R}_{\rm n}|} + \frac{(\vec{r}_i - \vec{R}_{\rm n})(\vec{\boldsymbol{\alpha}}_i \cdot (\vec{r}_i - \vec{R}_{\rm n}))}{|\vec{r}_i - \vec{R}_{\rm n}|^3} \Big] \cdot \vec{P}_{\rm n} \,.$$

Nuclear recoil effect in the Breit approximation

In the center-of-mass frame, using

$$\vec{P}_{\rm n} = -\sum_k \vec{p}_k \,,$$

and replacing $\vec{r}_i - \vec{R}_{\rm n} \to \vec{r}_i$, we get

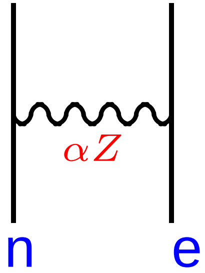
$$V_{\rm B} = -\frac{\alpha Z}{2M} \sum_{i,k} \Big[\frac{\vec{\boldsymbol{\alpha}}_i}{r_i} + \frac{\vec{r}_i(\vec{\boldsymbol{\alpha}}_i \cdot \vec{r}_i)}{r_i^3} \Big] \cdot \vec{p}_k \,.$$

The total nuclear recoil operator in the Breit approximation *(V.M. Shabaev, Theor. Math. Phys., 1985; Sov. J. Nucl. Phys., 1988; C.W. Palmer, J. Phys. B, 1987)*:

$$H = \frac{1}{2M} \sum_{i,k} \Big[\vec{p}_i \cdot \vec{p}_k - \frac{\alpha Z}{r_i} \Big(\vec{\alpha}_i + \frac{(\vec{\alpha}_i \cdot \vec{r}_i)\vec{r}_i}{r_i^2} \Big) \cdot \vec{p}_k \Big] \,.$$

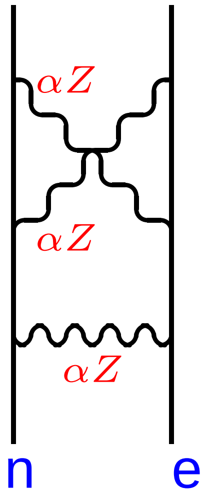
Fully relativistic theory of the nuclear recoil effect

The Breit approximation in terms of the Feynman diagrams:



Fully relativistic theory of the recoil effect in a H-like atom:

A typical diagram:



To get a closed formula for the recoil correction to all orders in αZ we need to sum all these diagrams.

Fully relativistic theory of the nuclear recoil effect

First formulation of the problem: *L.N. Labzowsky, 1972.*

First analysis of all relevant Feynman diagrams: *M.A. Braun, JETP, 1973.*

Complete formula for the nuclear recoil effect in a H-like atom to first order in m/M and to all orders in αZ *(V.M. Shabaev, Theor. Math. Phys., 1985)*:

$$
\begin{aligned}
\Delta E &= \Delta E_{\rm L} + \Delta E_{\rm H} \\
\Delta E_{\rm L} &= \frac{1}{2M}\langle a|\Big[\vec{p}^2 - \frac{\alpha Z}{r}\Big(\vec{\alpha} + \frac{(\vec{\alpha}\cdot\vec{r})\vec{r}}{r^2}\Big)\cdot\vec{p}\Big]|a\rangle\,, \\
\Delta E_{\rm H} &= \frac{i}{2\pi M}\int_{-\infty}^{\infty} d\omega\,\langle a|\Big(\vec{D}(\omega) - \frac{[\vec{p},V_{\rm C}]}{\omega+i0}\Big)G(\omega+\varepsilon_a)\Big(\vec{D}(\omega) + \frac{[\vec{p},V_{\rm C}]}{\omega+i0}\Big)|a\rangle\,,
\end{aligned}
$$

where $D_k(\omega) = -4\pi\alpha Z\alpha_i D_{ik}(\omega)\,,\, D_{ik}(\omega,r)$ is the transverse part of the photon propagator in the Coulomb gauge, and $G(\omega) = \sum_n \frac{|n\rangle\langle n|}{\omega-\varepsilon_n(1-i0)}$ is the Coulomb Green function.

Fully relativistic theory of the nuclear recoil effect

Rederivations by other authors:

A.S. Yelkhovsky, arXiv, 1994;

K. Pachucki and H. Grotch, PRA 1995;

G.S. Adkins, S. Morrison, and J. Sapirstein, PRA, 2007.

Representation in a more compact form *(A.S. Yelkhovsky, JETP , 1996)*:

$$\Delta E = \frac{i}{2\pi M}\int_{-\infty}^{\infty} d\omega \, \langle a|[\vec{p} - \vec{D}(\omega)]G(\omega + E_a)[\vec{p} - \vec{D}(\omega)]|a\rangle \, .$$

Numerical evaluations:

A.N. Artemyev, V.M. Shabaev, V.A. Yerokhin, PRA, 1995; JPB, 1995;

V.M. Shabaev et al., PRA, 1998; Phys. Scr., 1999;

G.S. Adkins, S. Morrison, and J. Sapirstein, PRA, 2007.

Extention to many-electron atoms: *V.M. Shabaev, Sov. J. Nucl. Phys., 1988.*

Radiative nuclear recoil to all orders in αZ: *K. Pachucki, PRA, 1995.*

Fully relativistic theory of the nuclear recoil effect

Simple formulation of the QED theory of the recoil effect in atoms

(V.M. Shabaev, PRA, 1998)

In the Schrödinger representation and the Coulomb gauge, the Hamiltonian of the whole system is

$$
\begin{aligned}
H &= \int d\vec{x}\psi^{\dagger}(\vec{x})[\vec{\alpha}\cdot(-i\vec{\nabla}_{\vec{x}} - e\vec{A}(\vec{x})) + \beta m]\psi(\vec{x}) \\
&\quad + \frac{e^2}{8\pi}\int d\vec{x}d\vec{y}\,\frac{\rho_e(\vec{x})\rho_e(\vec{y})}{|\vec{x}-\vec{y}|} + \frac{1}{2}\int d\vec{x}[\vec{\mathcal{E}}_{\rm t}^2(\vec{x}) + \vec{\mathcal{H}}^2(\vec{x})] \\
&\quad + \frac{e|e|Z}{4\pi}\int d\vec{x}\,\frac{\rho_e(\vec{x})}{|\vec{x}-\vec{X}_{\rm n}|} + \frac{1}{2M}[\vec{P}_{\rm n} - |e|Z\vec{A}(\vec{X}_{\rm n})]^2 \\
&\quad - \vec{\mu}\cdot\vec{\mathcal{H}}(\vec{X}_{\rm n})\,,
\end{aligned}
$$

where the nucleus is considered as a nonrelativistic particle with mass M. The term $-\vec{\mu}\cdot\vec{\mathcal{H}}$ causes the hyperfine splitting of atomic levels and will be omitted.

Fully relativistic theory of the nuclear recoil effect

The total momentum of the system is given by

$$\vec{P} = \vec{P}_{\rm n} + \vec{P}_{\rm e} + \vec{P}_{\rm ph}\,,$$

where

$$\vec{P}_{\rm e} = \int d\vec{x}\,\psi^{\dagger}(\vec{x})(-i\vec{\nabla}_{\vec{x}})\psi(\vec{x})$$

is the electron-positron field momentum and

$$\vec{P}_{\rm ph} = \int d\vec{x}\,[\vec{\mathcal{E}}_{\rm t}(\vec{x}) \times \vec{\mathcal{H}}(\vec{x})]$$

is the electromagnetic field momentum. In the center-of-mass frame:

$$\vec{P}\Phi = (\vec{P}_{\rm n} + \vec{P}_{\rm e} + \vec{P}_{\rm ph})\Phi = 0\,.$$

Fully relativistic theory of the nuclear recoil effect

In the center-of-mass frame ($\vec{P} = 0$), using

$$\vec{P}_{\rm n} = -\vec{P}_{\rm e} - \vec{P}_{\rm ph} = -\int d\vec{x}\,\psi^\dagger(\vec{x})(-i\vec{\nabla}_{\vec{x}})\psi(\vec{x}) - \int d\vec{x}\,[\vec{\mathcal{E}}_{\rm t}(\vec{x}) \times \vec{\mathcal{H}}(\vec{x})]$$

and replacing $\vec{X}_{\rm n} \to 0$, we get

$$\begin{aligned} H \quad = \quad & \int d\vec{x}\,\psi^\dagger(\vec{x})[\vec{\alpha}\cdot(-i\vec{\nabla}_{\vec{x}} - e\vec{A}(\vec{x})) + \beta m]\psi(\vec{x}) \\ & + \frac{e^2}{8\pi}\int d\vec{x}\,d\vec{y}\,\frac{\rho_e(\vec{x})\rho_e(\vec{y})}{|\vec{x}-\vec{y}|} + \frac{1}{2}\int d\vec{x}\,[\vec{\mathcal{E}}_{\rm t}^2(\vec{x}) + \vec{\mathcal{H}}^2(\vec{x})] \\ & + \frac{e|e|Z}{4\pi}\int d\vec{x}\,\frac{\rho_e(\vec{x})}{|\vec{x}|} + \frac{1}{2M}\Big[-\int d\vec{x}\,\psi^\dagger(\vec{x})(-i\vec{\nabla}_{\vec{x}})\psi(\vec{x}) \\ & - \int d\vec{x}\,[\vec{\mathcal{E}}_{\rm t}(\vec{x}) \times \vec{\mathcal{H}}(\vec{x})] - |e|Z\vec{A}(0)\Big]^2 . \end{aligned}$$

Fully relativistic theory of the nuclear recoil effect

To zeroth order in α and to first order in m/M (but to all orders in αZ), the relativistic nuclear recoil operator is given by

$$\begin{aligned} H_M &= \frac{1}{2M} \int d\vec{x}\, \psi^\dagger(\vec{x})(-i\vec{\nabla}_{\vec{x}})\psi(\vec{x}) \int d\vec{y}\, \psi^\dagger(\vec{y})(-i\vec{\nabla}_{\vec{y}})\psi(\vec{y}) \\ &\quad - \frac{eZ}{M} \int d\vec{x}\, \psi^\dagger(\vec{x})(-i\vec{\nabla}_{\vec{x}})\psi(\vec{x})\vec{A}(0) + \frac{e^2 Z^2}{2M} \vec{A}^2(0)\,. \end{aligned}$$

To find the nuclear recoil effect for a state a, one should evaluate

$$\Delta E_a = \langle \Phi_a | H_M | \Phi_a \rangle\,.$$

The calculation can be performed by adding the Hamiltonian H_M to the standard QED Hamiltonian in the Furry picture. This results in appearing new lines and vertices in the Feynman rules.

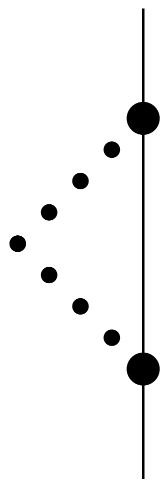
Fully relativistic theory of the nuclear recoil effect

Relativistic nuclear recoil effect for a H-like atom

The Coulomb nuclear recoil contribution is defined by the first term

$$\Delta E_a^{(\mathrm{C})} \quad = \quad \frac{1}{2M} \langle \Phi_a | \int d\vec{x}\, \psi^\dagger(\vec{x})(-i\vec{\nabla}_{\vec{x}})\psi(\vec{x}) \int d\vec{y}\, \psi^\dagger(\vec{y})(-i\vec{\nabla}_{\vec{y}})\psi(\vec{y}) | \Phi_a \rangle \,.$$

The corresponsing Feynman diagram:



Fully relativistic theory of the nuclear recoil effect

A simple evalution yields

$$\Delta E_a^{(\mathrm{C})} = \frac{1}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_n \frac{\langle a|\vec{p}|n\rangle\langle n|\vec{p}|a\rangle}{\omega - \varepsilon_n(1-i0)}\,.$$

Using the identities

$$\frac{1}{x \pm i0} = \pm\frac{\pi}{i}\delta(x) + \mathrm{P}\frac{1}{x}\,,$$

we get

$$\Delta E_a^{(\mathrm{C})} = \frac{1}{2M}\langle a|\vec{p}^{\,2}|a\rangle - \frac{1}{M}\sum_{\varepsilon_n<0} |\langle a|\vec{p}|n\rangle|^2\,.$$

Fully relativistic theory of the nuclear recoil effect

Alternative derivation of the Coulomb nuclear recoil contribution

We start with the nonrelativistic theory of the nuclear recoil effect for a many-electron atom

$$\begin{aligned}
\Delta E_a &= \frac{1}{2M}\Big\langle \Phi_a \Big| \Big(\sum_i \vec{p}_i\Big)^2 \Big| \Phi_a \Big\rangle \\
&= \frac{1}{2M}\Big\langle \Phi_a \Big| \sum_i \vec{p}_i^{\,2} \Big| \Phi_a \Big\rangle + \frac{1}{2M}\Big\langle \Phi_a \Big| \sum_{i\neq j} (\vec{p}_i \cdot \vec{p}_j) \Big| \Phi_a \Big\rangle
\end{aligned}$$

In the independent electron approximation, the wave function Φ_a is a one-determinant wave function:

$$\Phi_a(\vec{x}_1, ..., \vec{x}_N) = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \psi_{Pa_1}(\vec{x}_1) \cdots \psi_{Pa_N}(\vec{x}_N)$$

Fully relativistic theory of the nuclear recoil effect

Let us consider an atom with one electron over closed shells. We are interested in the nuclear recoil effect on the $v \to v'$ transition energy:

$$\Delta E_{v\to v'} = \frac{1}{2M}\langle v|\vec{p}^2|v\rangle - \frac{1}{2M}\langle v'|\vec{p}^2|v'\rangle - \Big[\frac{1}{M}\sum_c |\langle v|\vec{p}|c\rangle|^2 - \frac{1}{M}\sum_c |\langle v'|\vec{p}|c\rangle|^2\Big] .$$

For instance, in case of a B-like atom: $v = 2p_{3/2}$, $v' = 2p_{1/2}$, $c = 1s, 2s$,

$$\Delta E_{v\to v'} = \frac{1}{2M}\langle 2p_{3/2}|\vec{p}^2|2p_{3/2}\rangle - \frac{1}{2M}\langle 2p_{1/2}|\vec{p}^2|2p_{1/2}\rangle - \Big[\frac{1}{M}\sum_{c=1s,2s} |\langle 2p_{3/2}|\vec{p}|c\rangle|^2 - \frac{1}{M}\sum_{c=1s,2s} |\langle 2p_{1/2}|\vec{p}|c\rangle|^2\Big] .$$

Fully relativistic theory of the nuclear recoil effect

Extension to the Dirac theory:

$$\begin{aligned}\Delta E_{v\to v'} \quad = \quad & \frac{1}{2M}\langle 2p_{3/2}|\vec{p}^{\,2}|2p_{3/2}\rangle - \frac{1}{2M}\langle 2p_{1/2}|\vec{p}^{\,2}|2p_{1/2}\rangle \\ & -\Big[\frac{1}{M}\sum_{c=1s,2s}|\langle 2p_{3/2}|\vec{p}|c\rangle|^2 - \frac{1}{M}\sum_{c=1s,2s}|\langle 2p_{1/2}|\vec{p}|c\rangle|^2\Big] \\ & -\Big[\frac{1}{M}\sum_{\varepsilon_n<-mc^2}|\langle 2p_{3/2}|\vec{p}|n\rangle|^2 - \frac{1}{M}\sum_{\varepsilon_n<-mc^2}|\langle 2p_{1/2}|\vec{p}|n\rangle|^2\Big]\,.\end{aligned}$$

The last term describes the interaction of the valence electron with the negative-continuum Dirac electrons via coupling to the common dynamics with the nucleus.

Fully relativistic theory of the nuclear recoil effect

The one-transverse-photon nuclear recoil contribution is defined by the second term

$$\Delta E_a^{(\mathrm{tr1})} = -\frac{eZ}{M}\langle\Phi_a|\int d\vec{x}\,\psi^\dagger(\vec{x})(-i\vec{\nabla}_{\vec{x}})\psi(\vec{x})\vec{A}(0)|\Phi_a\rangle\,.$$

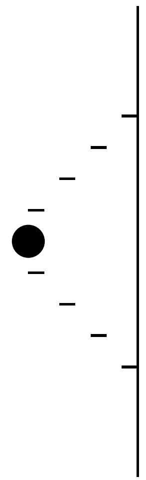
The corresponsing Feynman diagrams:

Fully relativistic theory of the nuclear recoil effect

The two-transverse-photon nuclear recoil contribution is defined by the third term

$$\Delta E_a^{(\mathrm{tr2})} = \frac{e^2 Z^2}{2M} \langle \Phi_a | \vec{A}^2(0) | \Phi_a \rangle \,.$$

The corresponsing Feynman diagram:



Fully relativistic theory of the nuclear recoil effect

Evalution of the one- and two-transverse-photon recoil contributions yields

$$\Delta E_a^{(\mathrm{tr1})} = -\frac{1}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\,\langle a|[\vec{p}\,G(\omega+\varepsilon_a)\,\vec{D}(\omega)+\vec{D}(\omega)\,G(\omega+\varepsilon_a)\,\vec{p}]|a\rangle\,,$$

$$\Delta E_a^{(\mathrm{tr2})} = \frac{1}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\,\langle a|\vec{D}(\omega)G(\omega+\varepsilon_a)\vec{D}(\omega)|a\rangle\,,$$

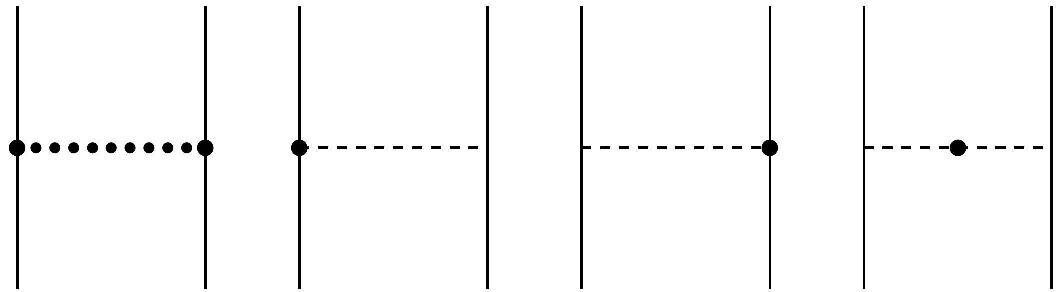
where $G(\omega)=\sum_n \frac{|n\rangle\langle n|}{\omega-\varepsilon_n(1-i0)}$ is the electron Green function and $D_k(\omega)=-4\pi\alpha Z\alpha_i D_{ik}(\omega)$.

The sum of all the contributions is given by

$$\Delta E_a^{(\mathrm{tot})} = \frac{1}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\,\langle a|[\vec{p}-\vec{D}(\omega)]G(\omega+\varepsilon_a)[\vec{p}-\vec{D}(\omega)]|a\rangle\,.$$

Fully relativistic theory of the nuclear recoil effect

Two-electron recoil contributions:



For a two-electron atom with the wave function

$$\Phi(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}} \sum_P (-1)^P \psi_{Pa}(\vec{x}_1)\psi_{Pb}(\vec{x}_2)$$

we get

$$\Delta E^{(\mathrm{int})} = \frac{1}{M} \sum_P (-1)^P \langle Pa|[\vec{p} - \vec{D}(\varepsilon_{Pa} - \varepsilon_a)]|a\rangle \langle Pb|[\vec{p} - \vec{D}(\varepsilon_{Pb} - \varepsilon_b)]|b\rangle \, .$$

Finite nuclear size effect

The nuclear charge distribution is usually approximated by the spherically-symmetric Fermi model:

$$\rho(r) = \frac{N}{1 + \exp[(r - c)/a]},$$

where the parameter a is generally fixed to be $a = 2.3/(4 \ln 3)$ fm and the parameters N and c are determined using the given value of $R = \langle r^2 \rangle^{1/2}$ and the normalization condition: $\int d\vec{r} \rho(r) = 1$. The potential induced by the nuclear charge distribution $\rho(r)$ is defined as

$$V_{\rm nuc}(r) = 4\pi\alpha Z \int_0^\infty dr' r^2 \rho(r') \frac{1}{r_>},$$

where $r_> = \max(\mathrm{r}, \mathrm{r}')$. The isotope field shift is obtained by calculations of the binding energies for the two isotopes and taking the corresponding energy difference.

Finite nuclear size effect

Finite nuclear size effect in H-like ions

In the range Z=1-100, with relative accuracy of $\sim 0.2\%$, *(V.M. Shabaev, J.Phys. B, 1993)*

$$\Delta E_{ns} = \frac{(\alpha Z)^2}{10n}[1 + (\alpha Z)^2 f_{ns}(\alpha Z)]\Big(2\frac{\alpha Z}{n}\frac{R_{\rm eff}}{(\hbar/mc)}\Big)^{2\gamma} mc^2\,,$$

where $\gamma = \sqrt{1-(\alpha Z)^2}$,

$$\begin{aligned} f_{1s}(\alpha Z) &= 1.380 - 0.162\alpha Z + 1.612(\alpha Z)^2\,, \\ f_{2s}(\alpha Z) &= 1.508 + 0.215\alpha Z + 1.332(\alpha Z)^2\,, \end{aligned}$$

and $R_{\rm eff}$ is an effective nuclear radius defined by

$$R_{\rm eff} = \Big\{\frac{5}{3}\langle r^2\rangle\Big[1 - \frac{3}{4}(\alpha Z)^2\Big(\frac{3}{25}\frac{\langle r^4\rangle}{\langle r^2\rangle^2} - \frac{1}{7}\Big)\Big]\Big\}^{1/2}.$$

Nuclear deformation effect

The nuclear deformation effect is evaluated by replacing the standard Fermi model for the nuclear charge distrubution by *(Yu.S. Kozhedub et al., PRA, 2008)*

$$\rho(r) = \frac{1}{4\pi} \int d\vec{n} \rho(\vec{r}) \,,$$

where $\rho(\vec{r})$ is the axially symmetric Fermi distribution:

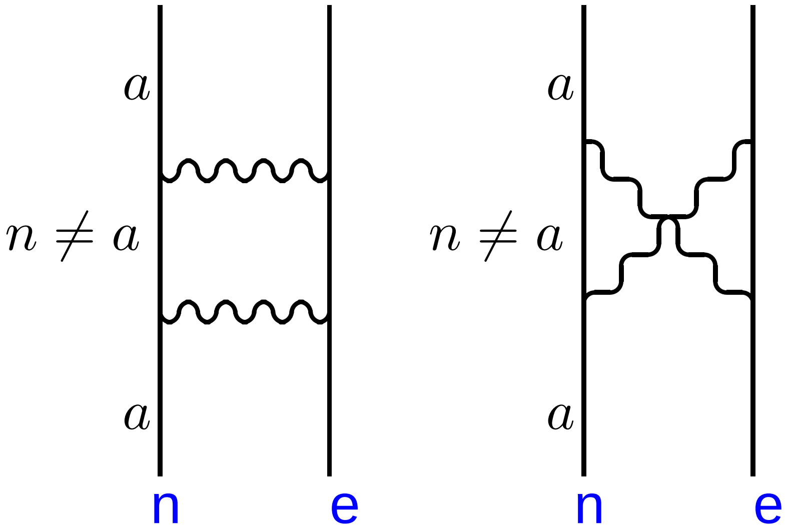
$$\rho(\vec{r}) = \frac{N}{1 + \exp[(r - r_0(1 + \beta_{20} Y_{20}(\theta) + \beta_{40} Y_{40}(\theta))/a]}$$

consistent with the normalization condition: $\int d\vec{r} \rho(\vec{r}) = 1$.

The difference between the nuclear size effect obtained with the deformed and spherically-symmetric Fermi models at the same rms radius is ascribed to the nuclear deformation effect.

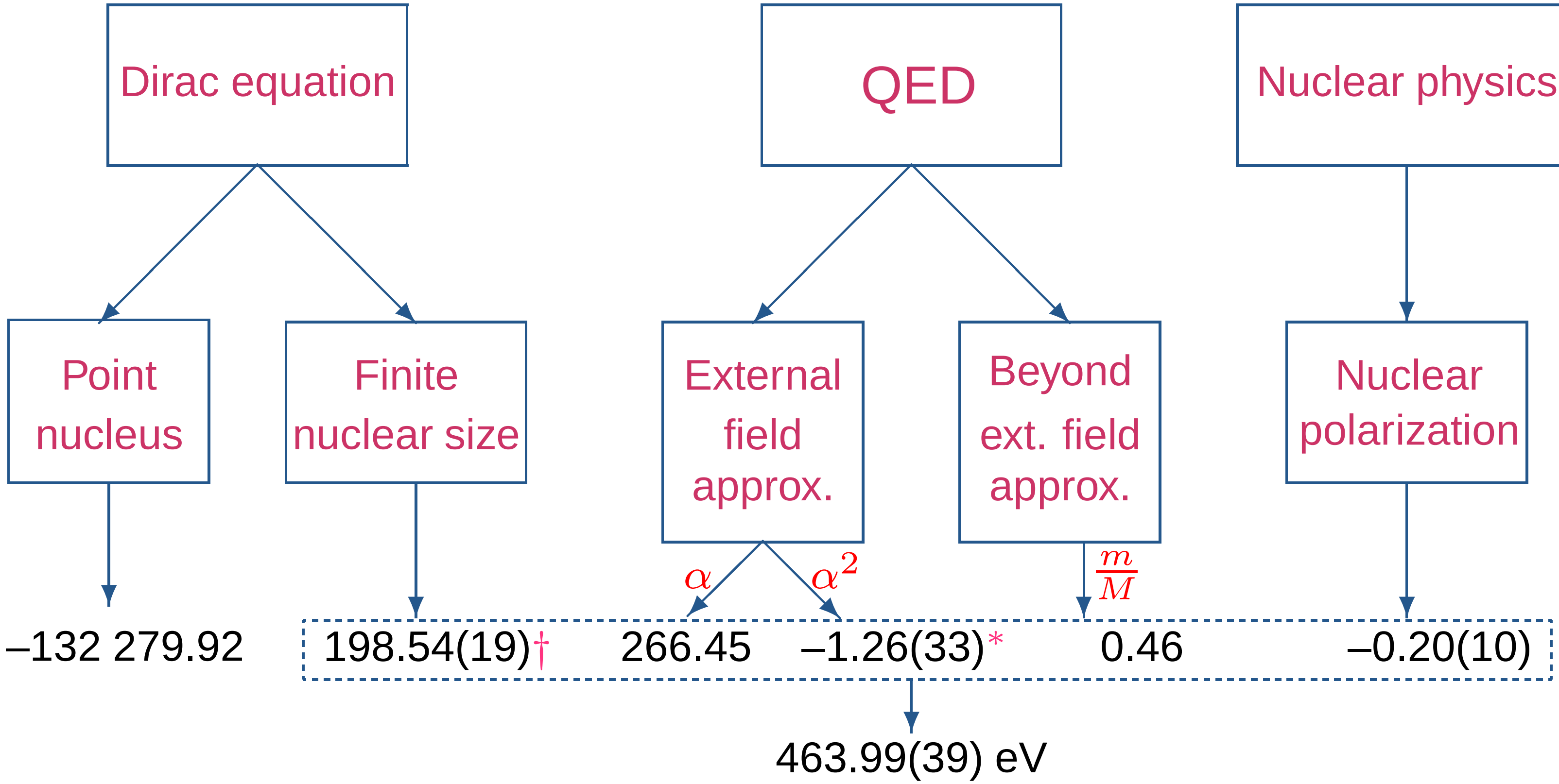
Nuclear polarization effect

The interaction between the electron and the nucleons causes the nucleus to make virtual transitions to excited states. This results in the increase of the binding energy of the electron.



Evaluation: *G. Plunien and G. Soff, PRA, 1995;*
A.V. Nefiodov, L.N. Labzowsky, G. Plunien, and G. Soff, PLA, 1996.

1s Lamb shift in H-like uranium, in eV



Experiment: 460.2(4.6) eV

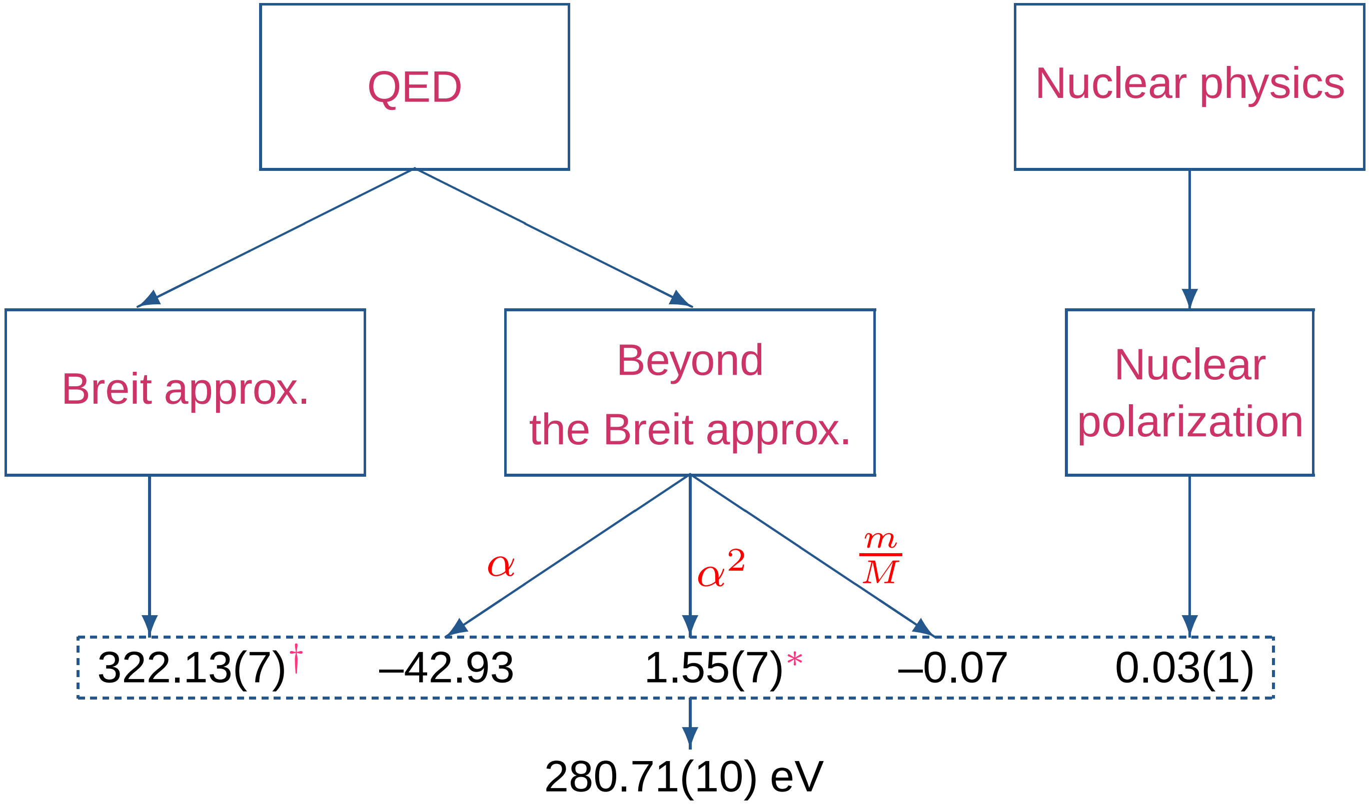
(A. Gumberidze, T. Stöhlker, D. Banas et al., PRL, 2005)

Test of QED: $\sim$ 2%

* V.A. Yerokhin, P. Indelicato, and V.M. Shabaev, PRL, 2006

† Y.S. Kozhedub, O.V. Andreev, V.M. Shabaev et al., PRA, 2008

$2p_{1/2}$-$2s$ *transition energy in Li-like uranium, in eV*



Experiment: 280.59(10) eV (J. Schweppe et al., PRL, 1991)
280.52(10) eV (C. Brandau et al., PRL, 2003)
280.645(15) eV (P. Beiersdorfer et al., PRL, 2005)

Test of QED: $\sim$ 0.2%

* V.A. Yerokhin, P. Indelicato, and V.M. Shabaev, PRL, 2006

† Y.S. Kozhedub, O.V. Andreev, V.M. Shabaev et al., PRA, 2008

Isotope shift in Li-like neodymium

Individual contributions to the isotope shifts for the $2p_{1/2} - 2s$ and $2p_{3/2} - 2s$ transitions in Li-like neodymium, ${}^{150,142}\mathrm{Nd}^{57+}$, (in meV) with ${}^{150,142}\delta\langle r^2\rangle = 1.36\,\mathrm{fm}^2$ *(N.A. Zubova et al., PRA, 2014)*.

Contribution	$2\mathrm{p}_{1/2} - 2\mathrm{s}$	$2\mathrm{p}_{3/2} - 2\mathrm{s}$
Field shift: non-QED	–42.57	–44.05
Mass shift: non-QED	1.30	1.50
Field shift: QED	0.22	0.24
Mass shift: QED	0.33	0.30
Nuclear polarization	0.36	0.33
Nuclear deformation	0.27	0.28
Total theory	–40.1(2)	–41.4(2)
Experiment *(C. Brandau et al., PRL, 2008)*	–40.2(3)(6)	–42.3(12)(20)

Nuclear recoil effect on the bound-electron g factor

The g factor of an atom can be defined as a proportionality coefficient in the Zeeman splitting of atomic levels:

$$\Delta E = g\,(|e|\hbar/2m_e)BM_z\,.$$

Formula for the nuclear recoil effect on the g-factor of a H-like atom to first order in m/M and to all orders in αZ *(V.M. Shabaev, PRA, 2001)*:

$$\begin{aligned}\Delta g_{\rm nuc.rec.} \quad &= \quad \frac{1}{\mu_0 m_a}\frac{i}{2\pi M}\int_{-\infty}^{\infty} d\omega\, \Bigg[\frac{\partial}{\partial B}\langle a|[\vec{p}-\vec{D}(\omega)+e\vec{A}_{\rm cl}] \\ &\times G(\omega+\varepsilon_a)[\vec{p}-\vec{D}(\omega)+e\vec{A}_{\rm cl}]|a\rangle\Bigg]_{B=0}\,,\end{aligned}$$

where it is implied that all quantities are calculated in the presence of the magnetic field B.

Nuclear recoil effect on the bound-electron g factor

For the practical calculations, the nuclear recoil effect can be represented by a sum of a lower-order term and a higher-order term, $\Delta g_{\rm nuc.rec.} = \Delta g^{\rm (L)}_{\rm nuc.rec.} + \Delta g^{\rm (H)}_{\rm nuc.rec.}$, where

$$\begin{aligned}
\Delta g^{\rm (L)}_{\rm nuc.rec.} &= \frac{1}{\mu_0 m_a}\frac{1}{2M}\left[\frac{\partial}{\partial B}\langle a|\Big(\vec{p}^2 - 2\vec{p}\cdot\vec{D}(0)\Big)|a\rangle\right]_{B=0} \\
&\quad -\frac{1}{m_a}\frac{m}{M}\langle a|\Big([\vec{r}\times\vec{p}]_z - \frac{\alpha Z}{2r}[\vec{r}\times\vec{\alpha}]_z\Big)|a\rangle_{B=0}\,, \\
\Delta g^{\rm (H)}_{\rm nuc.rec.} &= \frac{1}{\mu_0 m_a}\frac{i}{2\pi M}\int_{-\infty}^{\infty} d\omega\,\left[\frac{\partial}{\partial B}\langle a|\Big(\vec{D}(\omega) - \frac{[\vec{p},V]}{\omega+i0}\Big)\right. \\
&\quad \left.\times G(\omega+\varepsilon_a)\Big(\vec{D}(\omega) + \frac{[\vec{p},V]}{\omega+i0}\Big)|a\rangle\right]_{B=0}.
\end{aligned}$$

Numerical evaluation: *V.M. Shabaev and V.A. Yerokhin, PRL, 2002.*

Nuclear size effect on the g factor of H-like ions

Finite nuclear size correction for an ns state to the lowest order in αZ *(S.G. Karshenboim, PLA, 2000)*:

$$\Delta g_{\rm nuc.size} = \frac{8}{3n^3}(\alpha Z)^4 m^2 \langle r^2 \rangle_{\rm nuc} \,.$$

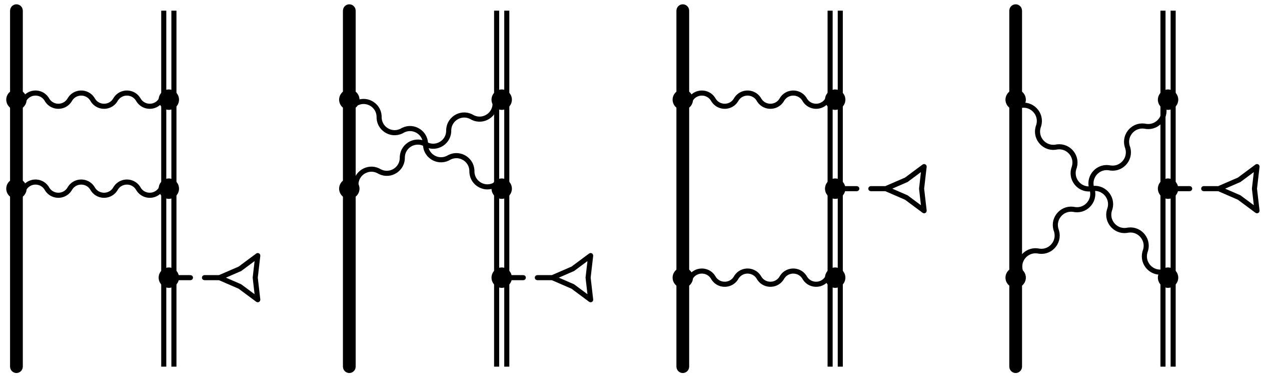
To two lowest orders in αZ *(D.A. Glazov and V.M. Shabaev, PLA, 2002)*:

$$\begin{aligned} \Delta g_{\rm nuc.size} \quad &= \quad \frac{8}{3n^3}(\alpha Z)^4 m^2 \langle r^2 \rangle_{\rm nuc} \Bigg[1 + (\alpha Z)^2 \Bigg(\frac{1}{4} + \frac{12n^2 - n - 9}{4n^2(n+1)} \\ &+ 2\psi(3) - \psi(2+n) - \frac{\langle r^2 \ln(2\alpha Z m r/n) \rangle_{\rm nuc}}{\langle r^2 \rangle_{\rm nuc}} \Bigg) \Bigg] \,. \end{aligned}$$

where $\psi(x) = \frac{d}{dx} \ln \Gamma(x)$.

Nuclear polarization effect on the g factor of H-like ions

The nuclear polarization corrections to the g factor of a H-like ion are defined by the Feynman diagrams:



Evaluations: *A.V. Nefiodov et al., PLB, 2003; A.V. Volotka and G. Plunien, PRL, 2014.*

Nuclear magnetic susceptibility correction to the bound-electron g factor: *U.D. Jentschura, A. Czarnecki, K. Pachucki, and V.A. Yerokhin, IJMS, 2006.*

g factor of H-like ions

g factor of $^{28}\mathrm{Si}^{13+}$

Dirac value (point nucleus)	1.993 023 571 6
Free QED	0.002 319 304 4
Binding QED [1]	0.000 005 855 8(17)
Recoil [2]	0.000 000 205 8(1)
Nuclear size	0.000 000 020 5
Total theory	1.995 348 958 0(17)
Experiment [3]	1.995 348 959 10(7)(7)(80)

[1] *K. Pachucki et al., PRA, 2005; V.A. Yerokhin et al., PRL, 2002.*

[2] *V.M. Shabaev and V.A. Yerokhin, PRL, 2002; K. Pachucki, PRA 2008.*

[3] *S. Sturm et al., PRL, 2011; PRA, 2013.*

These experiment and theory provide to date the most accurate test of bound-state QED with middle-Z ions.

g factor of Li-like ions

g factor of $^{28}\mathrm{Si}^{11+}$

Dirac value (point nucleus)	1.998 254 751
One-electron QED	0.002320527(1)
Screened QED	-0.000000236(5)
Interelectronic int.	0.000 314809(6)
Nuclear recoil	0.000 000 039(1)
Nuclear size	0.000 000 003
Total theory [1]	2.000 889 892(8)
Experiment [2]	2.000 889 890(2)

[1] *A.V. Volotka et al., PRL, 2014.*
[2] *A. Wagner et al., PRL, 2013.*

These experiment and theory provide the most stringent test of many-electron bound-state QED in a magnetic field.

Isotope shift of the g factor of H-like ions

Isotope shift of the g factor of H-like calcium: $^{40}\mathrm{Ca}^{19+} - \ ^{48}\mathrm{Ca}^{19+}$

Nuclear recoil: non-QED $\sim m/M$	0.000000048657
Nuclear recoil: non-QED $\sim (m/M)^2$	$-0.000000000026(2)$
Nuclear recoil: QED $\sim m/M$	0.000000000904
Nuclear recoil: QED $\sim \alpha(m/M)$	$-0.000000000038(3)$
Finite nuclear size	$0.000000000032(75)$
Total theory	$0.000000049529(75)$

The current theoretical uncertainty is about 8% of the QED nuclear recoil contribution.

Isotope shift of the g factor of Li-like ions

Calculations for low-Z Li-like ions ($Z \leq 12$) including the lowest-order relativistic and radiative corrections: *Zong-Chao Yan, PRL, 2001; JPB, 2002*.

New calculations

Isotope shift of the g-factor of Li-like calcium: $^{40}\mathrm{Ca}^{17+} - {}^{48}\mathrm{Ca}^{17+}$

Nuclear recoil: one-electron non-QED	$0.000000012240(1)$
Nuclear recoil: interelectronic int.	$-0.000000002051(22)$
Nuclear recoil: QED $\sim m/M$	$0.000000000123(12)$
Nuclear recoil: QED $\sim \alpha(m/M)$	$-0.000000000009(1)$
Finite nuclear size	$0.000000000004(9)$
Total theory	$0.000000010305(27)$

This study will provide the first test of QED beyond the Furry picture with highly charged ions.

Conclusion

- The QED calculations of the isotope shifts in highly charged ions are required by the current and near future experiments.
- The measurements and the calculations of the isotope shifts in highly charged ions provide an effective tool for determination of the nuclear charge radii.
- The study of the isotope shifts with highly charged ions can give a unique access to tests of QED at strong coupling regime beyond the Furry picture.