Calculations of the g factor and the hyperfine structure of heavy ions

Dmitry A. Glazov, Andrey V. Volotka, Vladimir M. Shabaev,
Ilja I. Tupitsyn, Günter Plunien

St. Petersburg State University

Institut für Theoretische Physik, TU Dresden

Outline

g factor of highly-charged ions

- Motivation for study
- Determination of α
  - Free-electron v.s. bound-electron g factor
  - Li-like ions
  - B-like ions
- Developements
  - Interelectronic interaction
  - QED corrections

Hyperfine splitting in highly-charged ions

- H-like ions
- Li-like ions
- B-like ions

Conclusion

Measurements of the bound-elecron g factor

$$g = -\langle \mu_z \rangle / \mu_{\mathrm{B}} \langle J_z \rangle ,$$

Mainz-GSI collaboration, HITRAP project

Single ion is cooled and trapped in the Penning trap.

Experimentally measured value:

$$\frac{\omega_L}{\omega_c} = \frac{g}{2} \frac{|e|}{q} \frac{m_{\mathrm{ion}}}{m_e}$$

2000: $^{12}\mathrm{C}^{5+}$

[N. Hermanspahn et al., PRL, 2000], [H. Häffner et al., PRL, 2000]

2004: $^{16}\mathrm{O}^{7+}$

[J. L. Verdú et al., PRL, 2004]

in progress: Ar, Ca

planned: Pb, U

Bound-elecron g factor and the electron mass

g factor of $^{12}C^{5+}$

Dirac value (point nucleus)	1.998 721 354 39(1)
Free QED	0.002 319 304 37(1)
Binding QED [1]	0.000 000 843 40(3)
Recoil [2]	0.000 000 087 62
Nuclear size	0.000 000 000 41
Total theory	2.001 041 590 18(3)
Experiment [3]	2.001 041 596 3(10)(44)

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

[2] *V. M. Shabaev, PRA, 2001; V.M. Shabaev and V.A. Yerokhin, PRL, 2002.*

[3] *H. Häfner et al., PRL, 2000.*

Determination of the electron mass: m_e = 0.000 548 579 909 32(29) u.

Test of QED in heavy ions

$$g = g_{\mathrm{D}}(\alpha Z) + \Delta g_{\mathrm{QED}}(\alpha, \alpha Z) + \Delta g_{\mathrm{nuc}}$$

$$\alpha = 1/137.036... - \text{fine structure constant}$$

$$Z - \text{nuclear charge}$$

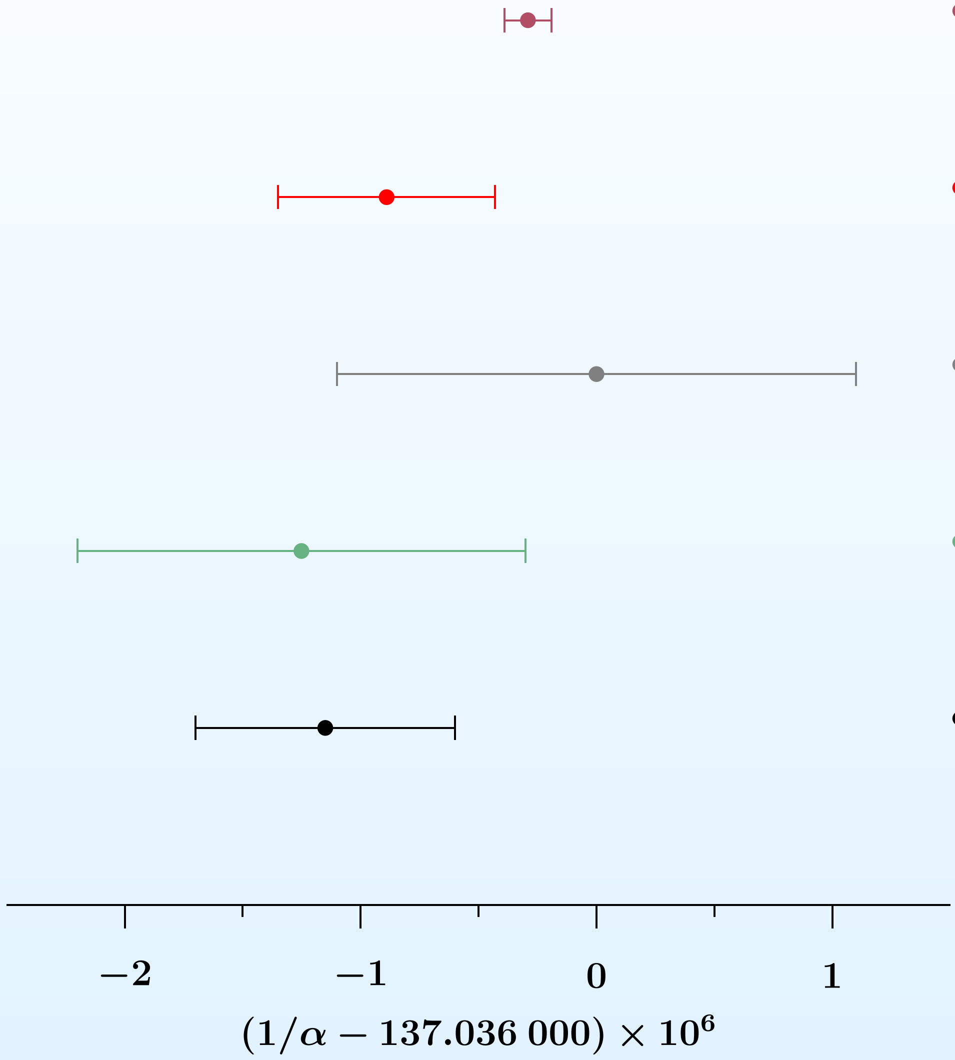
$$V_{\mathrm{nuc}}(r) = -\frac{\alpha Z}{r}$$

Expansion in α is always employed.

Low-Z systems: $\alpha Z \ll 1 \longrightarrow$ expansion in αZ.

High-Z systems: $\alpha Z \sim 1 \longrightarrow$ no expansion in αZ.
Furry picture: V_{nuc} is taken into account to all orders.
Strong-field regime of QED.

Present status of α determination



- $1/\alpha = 137.035\ 999\ 68(12) \quad \delta\alpha/\alpha = 0.7 \cdot 10^{-9}$
  CODATA 2006
- $1/\alpha = 137.035\ 999\ 11(46) \quad \delta\alpha/\alpha = 3.3 \cdot 10^{-9}$
  CODATA 2002
- $1/\alpha = 137.036\ 000\ 00(110)$
  transition frequencies in Cs
  [V. Gerginov et al., PRA **73**, *032504 (2006)]*
- $1/\alpha = 137.035\ 998\ 78(91)$
  transition frequencies in Rb
  [P. Cladé et al., PRL **96**, *033001 (2006)]*
- $1/\alpha = 137.035\ 998\ 80(52)$
  free-electron g factor (1987)
  [R. S. Van Dyck et al., PRL **59**, *26 (1987)]*

Free-electron g factor

$$g_{\text{free}} = 2\left(1 + \frac{\alpha}{\pi}A^{(2)} + \left(\frac{\alpha}{\pi}\right)^2 A^{(4)} + \ldots\right)$$

$$\frac{\mathrm{d}g_{\text{free}}}{\mathrm{d}\alpha} = \frac{1}{\pi}$$

$$\frac{\delta\alpha}{\alpha} = 2\left(\frac{\alpha}{\pi}\right)^{-1}\frac{\delta g_{\text{free}}}{g_{\text{free}}} = 861.022\ldots \times \frac{\delta g_{\text{free}}}{g_{\text{free}}}$$

$$\frac{\delta g_{\text{free}}^{\text{exp}}}{g_{\text{free}}} = 0.75 \times 10^{-12} \longrightarrow \frac{\delta\alpha}{\alpha} = 0.7 \times 10^{-9}$$

$g_{\text{free}}^{\text{exp}}$ = 2.002 319 304 361 7(15) $\longrightarrow 1/\alpha$ = 137.035 999 71(10)
$g_{\text{free}}^{\text{exp}}$ = 2.002 319 304 361 5(6) $\longrightarrow 1/\alpha$ = 137.035 999 08(5)

[G. Gabrielse et al., PRL, 2006], [D. Hanneke et al., PRL, 2008]

Bound-electron g factor

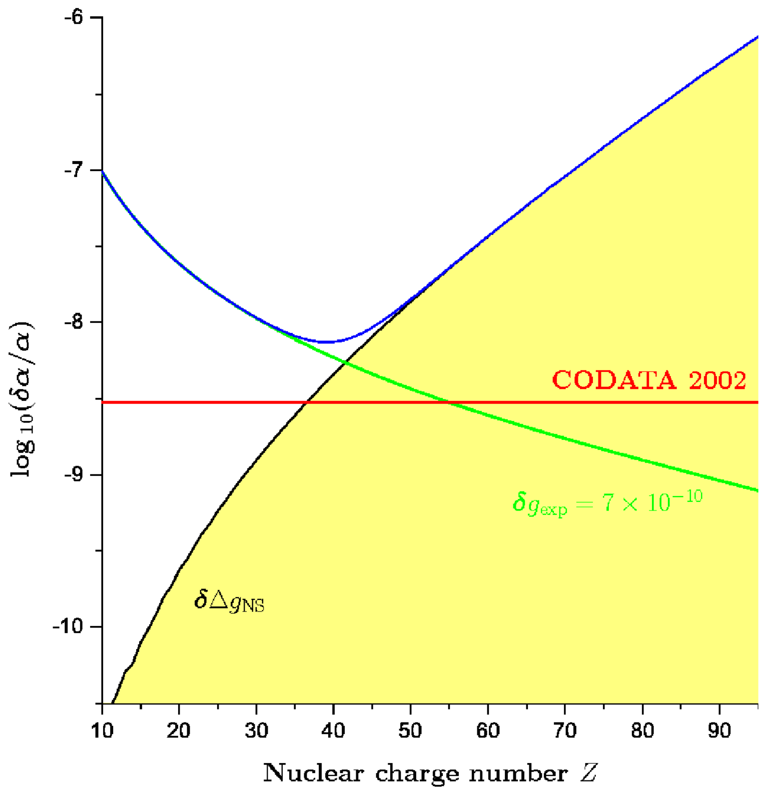
$$g_{1s} = \frac{2}{3}\left(2\sqrt{1-(\alpha Z)^2}+1\right) + \Delta g_{\mathrm{QED}} + \Delta g_{\mathrm{nuc}}$$

$$\frac{\mathrm{d}g_{1s}}{\mathrm{d}\alpha} = -\frac{4\alpha Z^2}{3\sqrt{1-(\alpha Z)^2}} \qquad \text{v.s.} \qquad \frac{\mathrm{d}g_{\mathrm{free}}}{\mathrm{d}\alpha} = \frac{1}{\pi}$$

$$\frac{\delta\alpha}{\alpha} = \frac{3\sqrt{1-(\alpha Z)^2}}{2(\alpha Z)^2}\,\frac{\delta g_{1s}}{g_{1s}} \qquad \text{v.s.} \qquad \frac{\delta\alpha}{\alpha} = 2\left(\frac{\alpha}{\pi}\right)^{-1}\frac{\delta g_{\mathrm{free}}}{g_{\mathrm{free}}}$$

$$\mathrm{Pb}\ \ (Z=82): \quad \delta g_{1s}^{\mathrm{exp}} = 0.7\times 10^{-9} \rightarrow \frac{\delta\alpha}{\alpha} = 1.3\times 10^{-9}$$

Nuclear effects



Measurements in heavy H-like ions at present experimental accuracy of 7×10^{-10} could compete with the ones in free electron for a precise determination of α.

However:

$\longrightarrow$ nuclear size and nuclear-polarization effects set the ultimate limit for $\delta g_{\rm th}$

$\longrightarrow$ the unsertainty due to the nuclear effect grows crucially with Z

Nuclear effects

One-electron relativistic value:

$$g = \frac{2\kappa}{j(j+1)} \frac{mc}{\hbar} \int_0^\infty \mathrm{d}r \, r^3 \, g(r) \, f(r) \to g_\mathrm{D} + \Delta g_\mathrm{NS}$$

Dirac wavefunction:

$$\Psi(r) = \begin{pmatrix} g(r)\Omega_{\kappa n}(\hat{r}) \\ i f(r)\Omega_{\overline{\kappa} n}(\hat{r}) \end{pmatrix}, \qquad \kappa = \left(j + \frac{1}{2}\right)(-1)^{j+l+\frac{1}{2}}$$

Dirac equation for bound electron:

$$\hbar c \frac{\mathrm{d}g(r)}{\mathrm{d}r} + \hbar c \frac{1+\kappa}{r} g(r) - \left(\varepsilon + mc^2 - V(r)\right) f(r) = 0$$

$$\hbar c \frac{\mathrm{d}f(r)}{\mathrm{d}r} + \hbar c \frac{1-\kappa}{r} f(r) + \left(\varepsilon - mc^2 - V(r)\right) g(r) = 0$$

Li-like ions

We have

$$\hbar c \frac{\alpha Z}{R_{\text{nuc}}} \gg |\varepsilon - mc^2| \approx \frac{(\alpha Z)^2}{2n^2} mc^2$$

$\Rightarrow$ the binding energy in the Dirac equation can be neglected for $r \leq R_{\text{nuc}}$.

$$\hbar c \, \frac{\mathrm{d}g(r)}{\mathrm{d}r} + \hbar c \, \frac{1+\kappa}{r} \, g(r) - \left(2mc^2 - V(r)\right) f(r) = 0$$
$$\hbar c \, \frac{\mathrm{d}f(r)}{\mathrm{d}r} + \hbar c \, \frac{1-\kappa}{r} \, f(r) + (-V(r)) \, g(r) = 0$$

This yields, in particular, for the states $1s$ and $2s$:

$$\begin{pmatrix} g_1(r) \\ f_1(r) \end{pmatrix} \approx C_{12} \begin{pmatrix} g_2(r) \\ f_2(r) \end{pmatrix} \quad \text{for} \quad r \lesssim R_{\text{nuc}}$$

Li-like ions

As a consequence, the parameter

$$\xi = \Delta g_{\rm NS}[(1s)^2 2s]/\Delta g_{\rm NS}[1s]$$

is rather insensitive to the nuclear model variations.
Let us introduce the specific difference

$$g' = g[(1s)^2 2s] - \xi g[1s]\,.$$

g' can be evaluated to much higher accuracy than g.

Advantage: elimination of the nuclear-size effect.

Drawback: large cancellation of the main α-dependent term.

$\longrightarrow$ significant reduction of the accuracy in α determination.

B-like ions

For high Z we have

$$\hbar c \frac{\alpha Z}{R_{\mathrm{nuc}}} \gg mc^2$$

$\Longrightarrow$ the electron rest energy can be neglected in the nuclear region.

$$\hbar c \, \frac{\mathrm{d}g(r)}{\mathrm{d}r} + \hbar c \, \frac{1+\kappa}{r} \, g(r) + V(r) f(r) = 0$$

$$\hbar c \, \frac{\mathrm{d}f(r)}{\mathrm{d}r} + \hbar c \, \frac{1-\kappa}{r} \, f(r) - V(r) g(r) = 0$$

Symmetry: $\kappa \longrightarrow -\kappa, \;\; g \longrightarrow f, \;\; f \longrightarrow -g$.
It yields, in particular, for the states $1s$ and $2p_{1/2}$:

$$\begin{pmatrix} g_1(r) \\ f_1(r) \end{pmatrix} \approx C_{12} \begin{pmatrix} f_2(r) \\ -g_2(r) \end{pmatrix} \quad \text{for} \quad r \lesssim R_{\mathrm{nuc}}$$

B-like ions

Let us introduce again

$$\xi = \Delta g_{\rm NS}[(1s)^2(2s)^2 2p_{1/2}]/\Delta g_{\rm NS}[1s]$$

and the specific difference

$$g' = g[(1s)^2(2s)^2 2p_{1/2}] - \xi g[1s]$$

g' can be evaluated to much higher accuracy than g.

Advantages:

elimination of the nuclear-size effect.

no significant cancellation of the main α-dependent term.

g factor of B-like Pb

The nuclear size effect on the g factor of B-like Pb was investigated numerically, including the $1/Z$ interelectronic interaction and the α/π QED corrections.

$$\xi = 0.009\,741\,6\,, \qquad \delta\xi = 0.000\,000\,25\,.$$

Uncertainty of g' due to the nuclear effects and the fine structure constant:

Contribution	$\delta g'/g'$
$1/\alpha = 137.035\,999\,11\,(46)$	8.7×10^{-10}
Nuclear size	2.9×10^{-10}
Nuclear polarization	1.0×10^{-10}

[V.M. Shabaev et al., PRL, 2006]

Developements

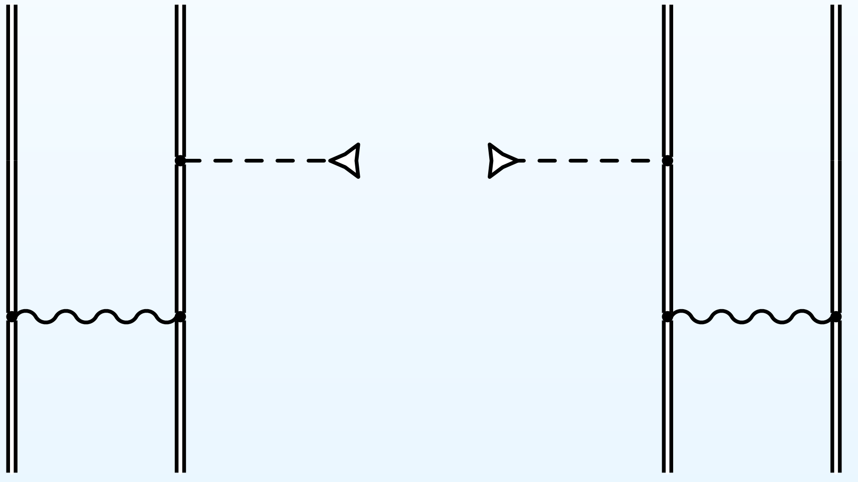
To achieve the required theoretical accuracy for the g factor necessitates a number of elaborate evaluations:

- Interelectronic interaction
  - ▷ $[1/Z]$ one-photon exchange
  - ▷ $[1/Z^2]$ two-photon exchange
  - ▷ higher orders: large-scale CI-DFS
- QED
  - ▷ $[\alpha]$ one-loop QED
    - + effective potential
    - + one-photon screening
  - ▷ $[\alpha^2]$ two-loop QED
    - + effective potential
  - ▷ $[\alpha^3]$ three-loop QED
- recoil effect
  - + effective potential
  - + QED corrections

Interelectronic interaction

$$\Delta g_{\mathrm{int}} = \frac{1}{Z}\,B(\alpha Z) + \frac{1}{Z^2}\,C(\alpha Z) + \ldots$$

$\boldsymbol{\frac{1}{Z}}$ **:**



$1/Z^2$ and higher:

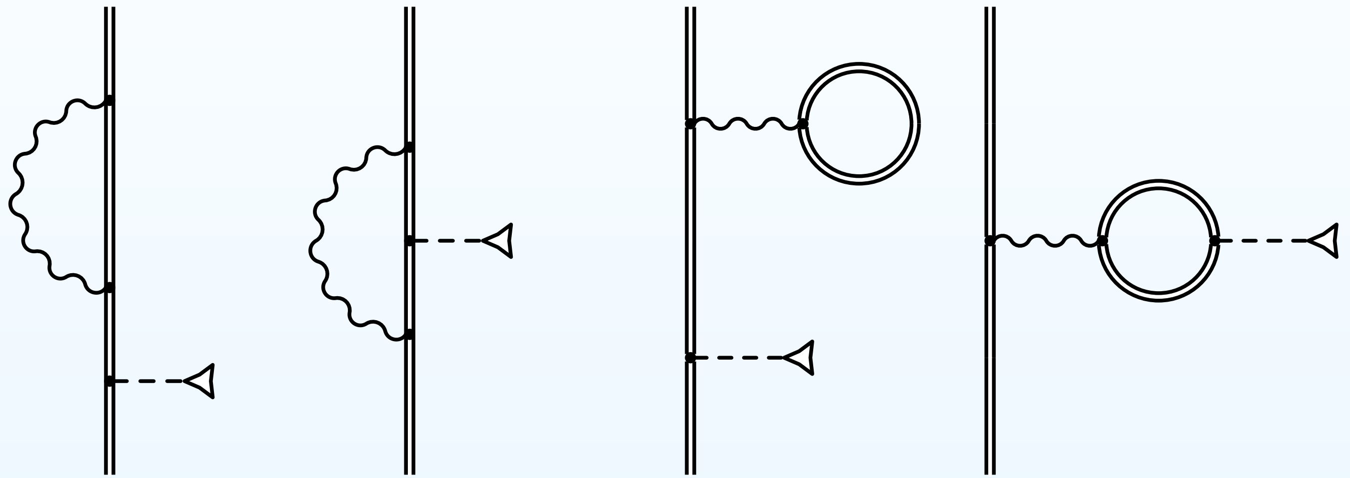
large-scale configuration-interaction Dirac-Fock-Sturm method

Basis: $12s\ 11p\ 10d\ 6f\ 4g\ 2h\ 1i$

[V. M. Shabaev et al., PRA, 2002], [D. A. Glazov et al., PRA, 2004]

One-loop QED corrections

$\frac{\alpha}{\pi}$:



$$\Delta g_{\rm QED} = \Delta g_{\rm SE} + \Delta g_{\rm VP} = 2\frac{\alpha}{\pi} A^{(2)}(\alpha Z)$$

$$A^{(2)}(\alpha Z) = \frac{1}{2} + \frac{(\alpha Z)^2}{12} + \ldots$$

[V. A. Yerokhin et al., PRA, 2004]

[R. N. Lee et al., PRA, 2005]

[K. Pachucki et al., PRA, 2005]

One-loop QED corrections: screening effect

Expansion in α and $1/Z$:

$$\Delta g_{\rm SQED} = \frac{\alpha}{\pi} \frac{(\alpha Z)^2}{Z} R(\alpha Z) + \ldots$$

$$\text{QED} \longrightarrow \hat{H}_{\rm eff} \sim \frac{\alpha}{\pi} A^{(2)}$$

[D. A. Glazov et al., PRA, 2004]

Effective potential approach:

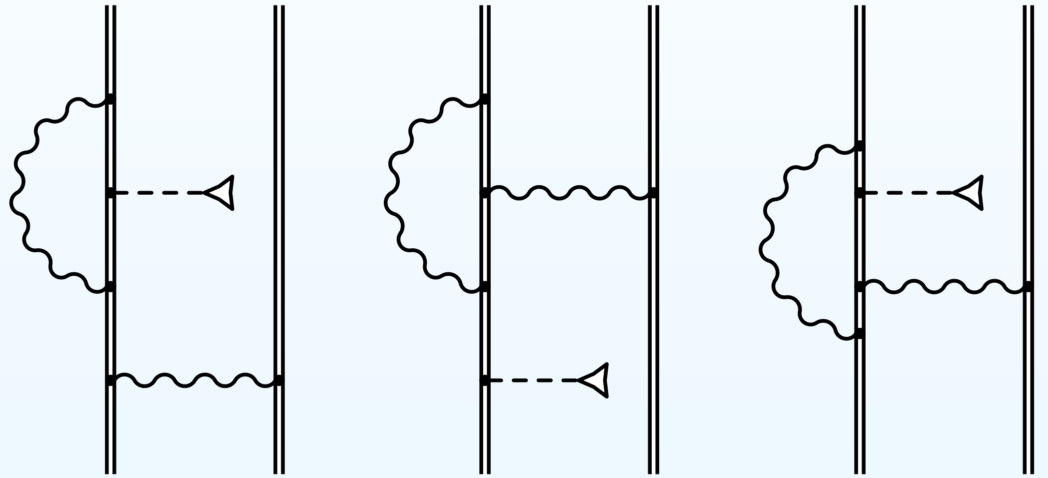
$$V_{\rm nuc}(r) \longrightarrow V_{\rm eff}(r) = V_{\rm nuc}(r) + V_{\rm scr}(r)$$

[D. A. Glazov et al., PLA, 2006]

One-loop QED corrections: screening effect

Rigorous QED evaluation of 27 diagrams like these:

$$\frac{1}{Z}\frac{\alpha}{\pi}:$$



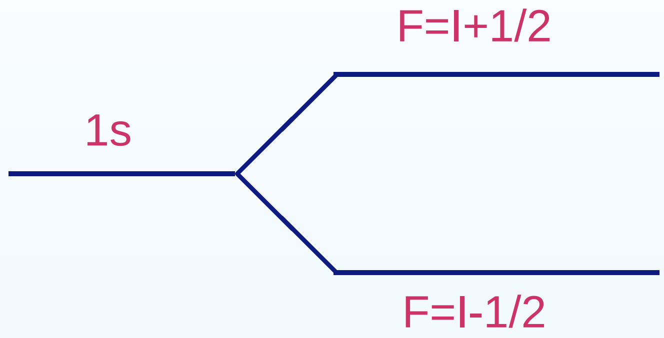
- The formulas were derived with the two-time Green function method.
- UV divergencies were separated within the "zero-potential" parts.
- The finite-basis-set method with DKB-splines was employed for the evaluation of the "many-potential" parts.
- New technique has been developed for dealing with IR divergencies.

g factor of Li-like Pb

Dirac value (point nucleus)	1.932 002 904
Interelectronic int.	0.002 140 7 (27)
QED, one-loop	0.002 411 7 (1)
QED, two-loop	-0.000 003 6 (5)
QED, screening	-0.000 001 6 (1)
Recoil	0.000 000 2 (3)
Nuclear size	0.000 078 6 (1)
Nuclear polarization	-0.000 000 04 (2)
Total theory	1.936 628 9 (28)

[A. V. Volotka et al., PRL, accepted]

Hyperfine splitting in H-like ions

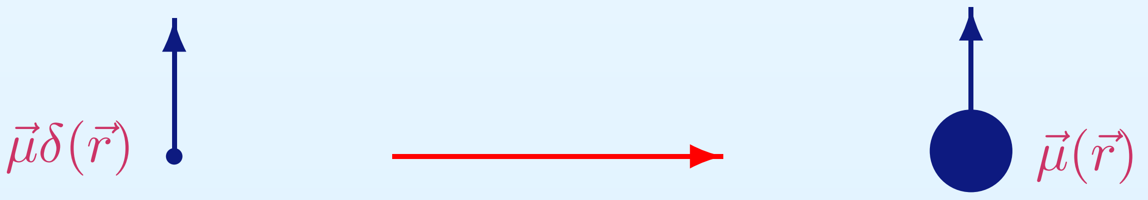


$$\Delta E = \Delta E_{\rm Dirac}(1-\delta)(1-\varepsilon) + \Delta E_{\rm QED}$$

δ — the nuclear charge distribution correction.

ε — the nuclear magnetization distribution correction =

= Bohr-Weisskopf effect:



Measurements of the hyperfine splitting in H-like ions.

I. Klaft et al., PRL, 1994:

$^{209}\mathrm{Bi}^{82+}$ $\Delta E^{\mathrm{exp}} = 5.0840(8)$ eV

J. Crespo Lopez-Urritia et al., PRL, 1996; PRA, 1998:

$^{165}\mathrm{Ho}^{66+}$ $\Delta E^{\mathrm{exp}} = 2.1645(6)$ eV

$^{185}\mathrm{Re}^{74+}$ $\Delta E^{\mathrm{exp}} = 2.7190(18)$ eV

$^{187}\mathrm{Re}^{74+}$ $\Delta E^{\mathrm{exp}} = 2.7450(18)$ eV

P. Seelig et al., PRL, 1998:

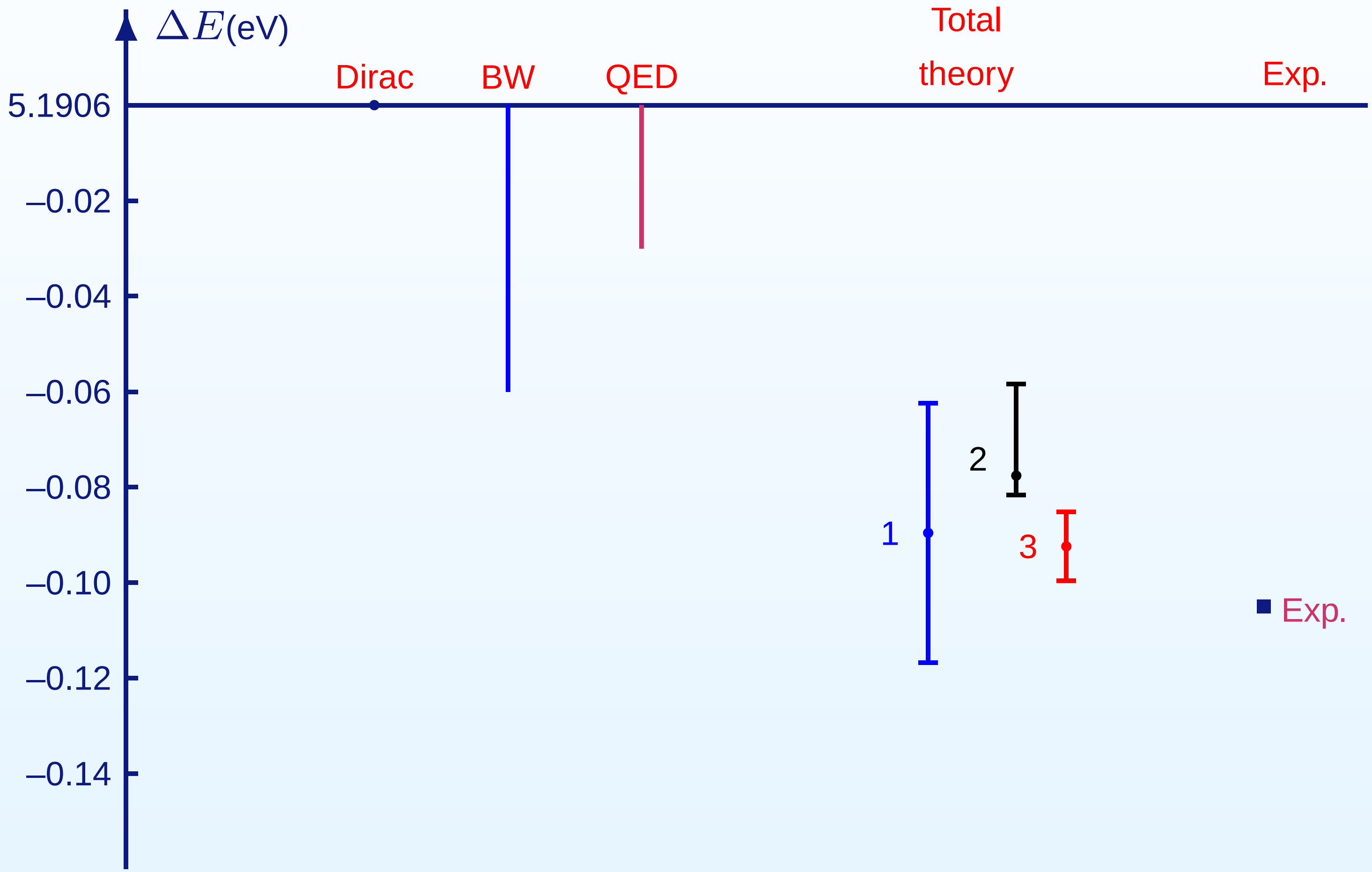
$^{207}\mathrm{Pb}^{81+}$ $\Delta E^{\mathrm{exp}} = 1.2159(2)$ eV

P. Beiersdorfer et al., PRA, 2001:

$^{203}\mathrm{Tl}^{80+}$ $\Delta E^{\mathrm{exp}} = 3.21351(25)$ eV

$^{205}\mathrm{Tl}^{80+}$ $\Delta E^{\mathrm{exp}} = 3.24410(29)$ eV

Hyperfine splitting in H-like Bi



[1] *V. M. Shabaev et al., PRA, 1997*

[2] *R. A. Sen'kov and V. F. Dmitriev, Nuc. Phys. A, 2002*

[3] *A. A. Elizarov et al., NIMB, 2005*

Exp.: *I. Klaft et al., PRL, 1994*

Hyperfine splitting in Li-like and B-like ions

Test of QED

Li-like ions *[V. M. Shabaev et al., PRL, 2001]*

$$\Delta' E = \Delta E[(1s)^2 2s] - \xi \Delta E[1s] \qquad \xi = \epsilon[(1s)^2 2s]/\epsilon[1s]$$

B-like ions *[N. S. Oreshkina et al., PLA, 2008]*

$$\Delta' E = \Delta E[(1s)^2 (2s)^2 2p_{1/2}] - \xi \Delta E[1s] \qquad \xi = \epsilon[(1s)^2 (2s)^2 2p_{1/2}]/\epsilon[1s]$$

$$\Delta E \sim \int_0^\infty \mathrm{d}r \, g(r) \, f(r) \, F(r)$$

Some ions are of interest in astrophysics:

[R. A. Sunyaev and E. M. Churazov, Pis'ma Astron. Zh., 1984]

[R. A. Sunyaev and D. N. Docenko, Astron. Lett., 2007]

Hyperfine splitting in Li-like Bi

Contributions to the $\Delta' E$

Dirac value (point nucleus)	-31.809
Interelectronic interaction	-29.75 (4)
QED	0.036
QED, screening	0.194 (4)
Total theory	-61.32 (4)

[H. Persson et al., PRL, 1996]
[V. M. Shabaev et al., PRL, 2001]
[J. Sapirstein and K. T. Cheng, PRA, 2001]

Screened QED diagrams: *[A. V. Volotka et al., PRL, accepted]*

Hyperfine splitting in B-like ions

$$\Delta E = E_{\rm F} \times \left[A(\alpha Z)(1-\delta)(1-\varepsilon) + \frac{1}{Z} B(\alpha Z) + \frac{1}{Z^2} C(Z,\alpha Z) + \Delta_{\rm QED} \right]$$

$$E_{\rm F} = \frac{\alpha(\alpha Z)^3}{18} \frac{m_e}{m_p} \frac{\mu}{\mu_N} \frac{2I+1}{2I} m_e c^2$$

Effect		^{45}Sc^{16+}	^{57}Fe^{21+}	^{209}Bi^{78+}
Dirac Value	A	1.04775	1.07472	2.58822
Nuclear size	δ	0.00004	0.00009	0.03341
Bohr-Weisskopf	ϵ	0.00001	0.00007	0.00307
e-e int.	B/Z	-0.29103	-0.24391	-0.24691
e-e int., h.o.	C/Z^2	0.01846	0.01294	0.00722
Screened QED	$\Delta_{\rm QED}$	0.00033	0.00029	-0.00489
Total [meV]	ΔE	1.7116(9)	0.11788(3)	258.09(35)

[N. S. Oreshkina et al., PLA, 2008], [A. V. Volotka et al., PRA, 2008]

Conclusion

Investigations of heavy ions provide:

- Accurate tests of QED in strong Coulomb field
- Determination of the fundamental constants
- Tests of nuclear models and determinaion of nuclear parameters