Many electron QED effects in the g factor of heavy ions

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Outline

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- Determination of α
  - Free-electron v.s. bound-electron g factor
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Bound-elecron g factor and the electron mass

Mainz-GSI collaboration | *HITRAP project*

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

Theory	2.001 041 590 18(3)	*Beier, Blundell, Czarnecki, Faustov, Indelicato, Jentschura, Karshenboim, Lindgren, Martynenko, Milstein, Pachucki, Sapirstein, Shabaev, Yerokhin*
Experiment	2.001 041 596 3(10)(44)	*[N. Hermanspahn et al., PRL, 2000], [H. Häffner et al., PRL, 2000]*

$$\frac{\omega_L}{\omega_c} = \frac{g}{2}\frac{|e|}{q}\frac{m_{\rm ion}}{m_e} \rightarrow m_e = 0.000\,548\,579\,909\,32(29)\mathrm{u}.$$

2004: $^{16}\mathrm{O}^{7+}$ *[J. L. Verdú et al., PRL, 2004]*

in progress: Si, Ca

planned: Pb, U

Test of QED in heavy ions

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

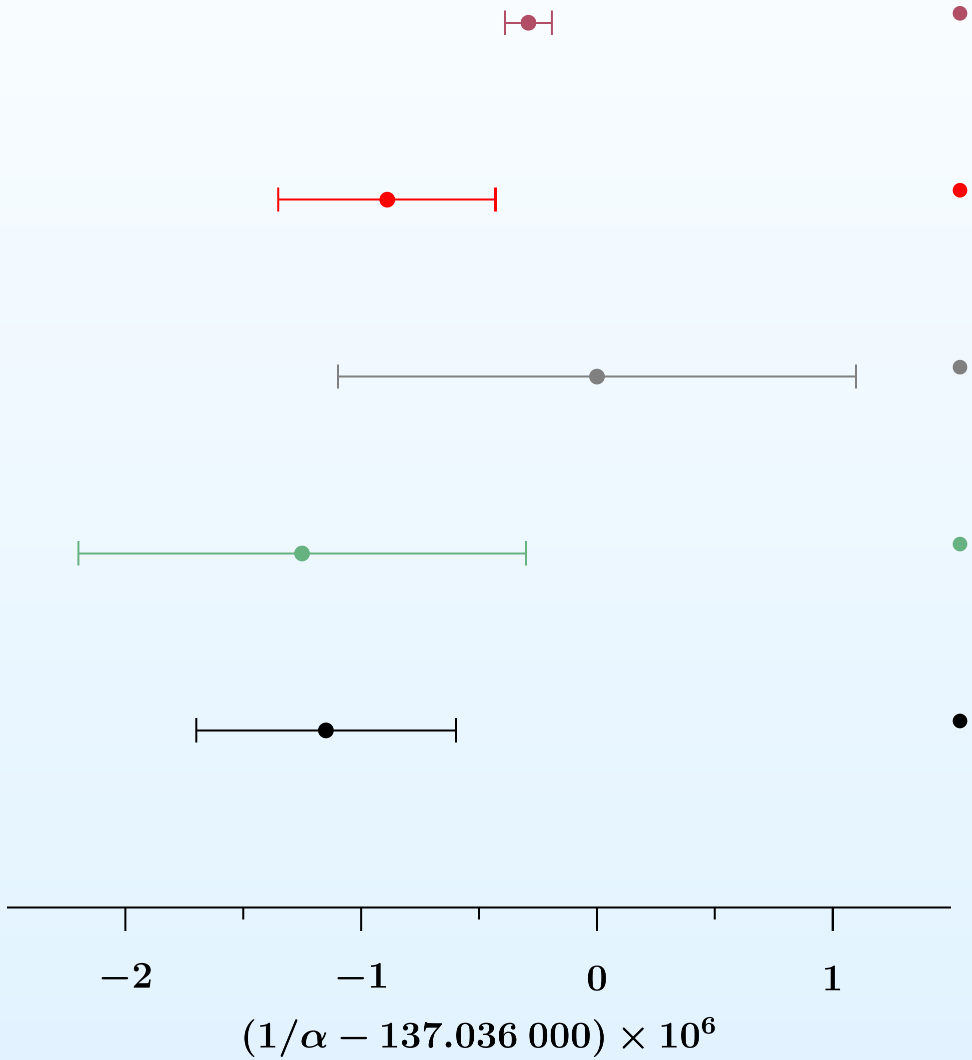
$$\alpha = 1/137.036... - \text{fine structure constant}$$
$$Z - \text{nuclear charge}$$
$$V_{\rm nuc}(r) = -\frac{\alpha Z}{r}$$

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: $V_{\rm nuc}$ 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

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

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

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

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

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

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

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

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

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

But

δg^{th} is limited by the nuclear size and structure

Nuclear size effect

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:

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

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

Li-like ions

We have

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

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

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

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

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

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

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

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

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

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]

Theoretical status

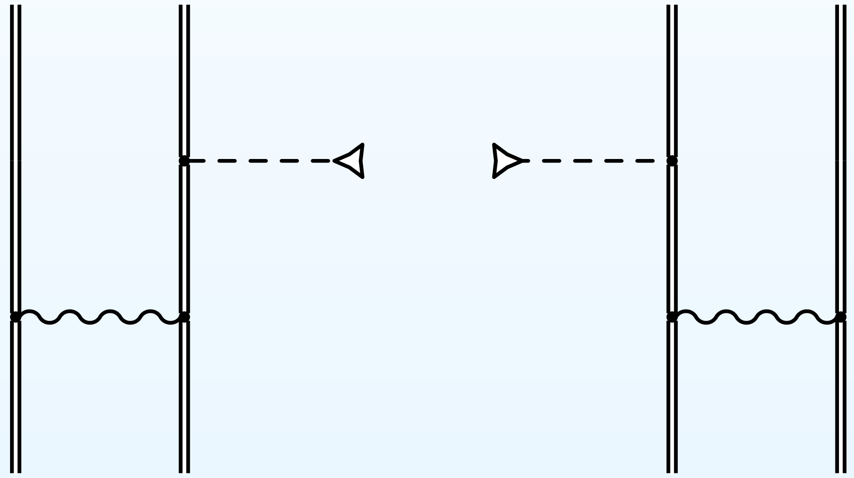
To achieve the required theoretical accuracy for the g factor necessitates a number of elaborate evaluations:

- 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

$$\Delta g_{\rm int} = \frac{1}{Z} B(\alpha Z) + \frac{1}{Z^2} C(\alpha Z) + \dots$$

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



$1/Z^2$ and higher:

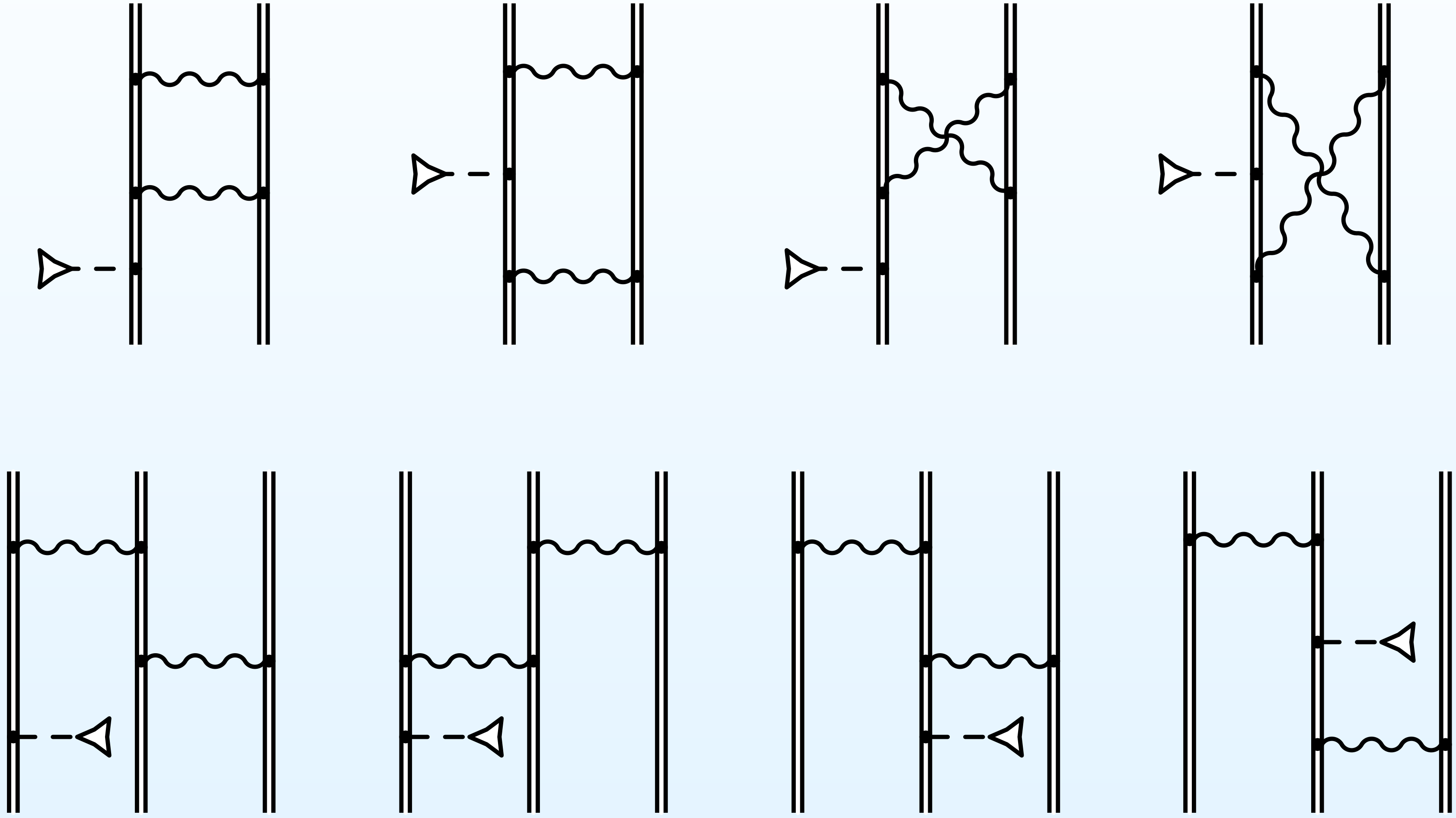
large-scale configuration-interaction Dirac-Fock-Sturm method

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

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

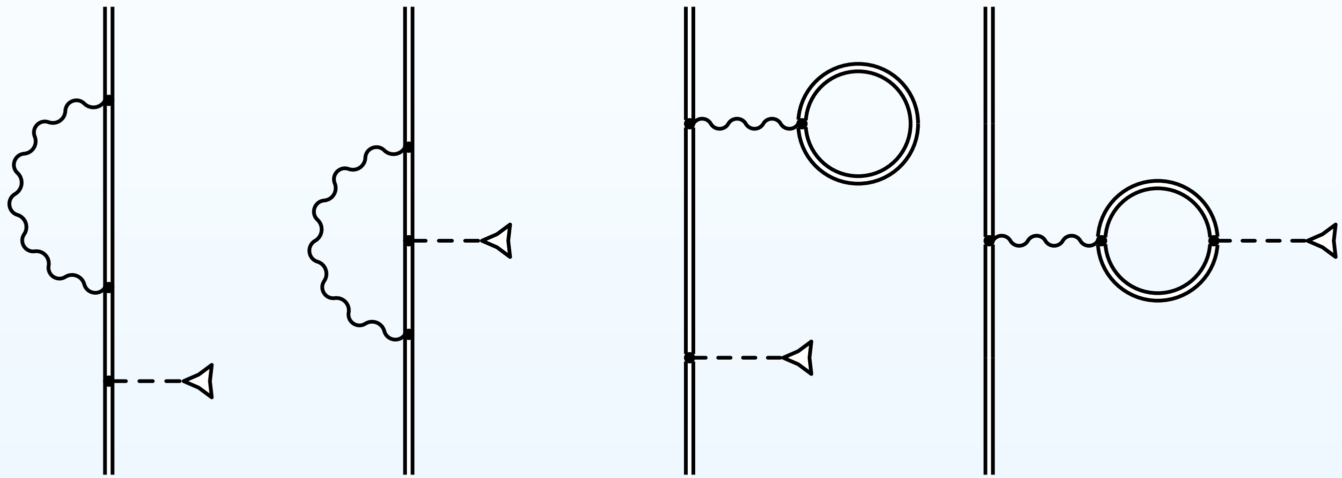
Interelectronic interaction

Two-photon exchange



One-loop QED corrections

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



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

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

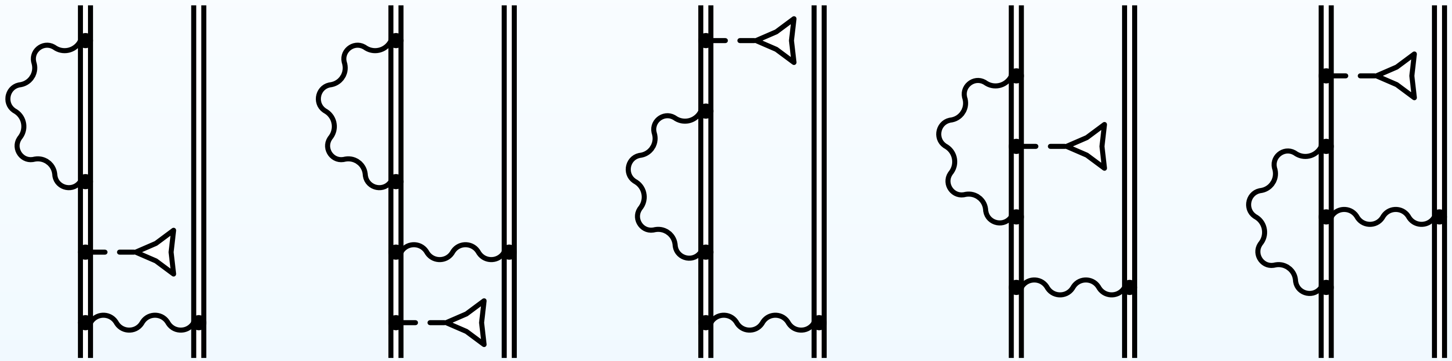
To all orders in αZ:

[V. A. Yerokhin et al., PRA, 2004], [K. Pachucki et al., PRA, 2005]

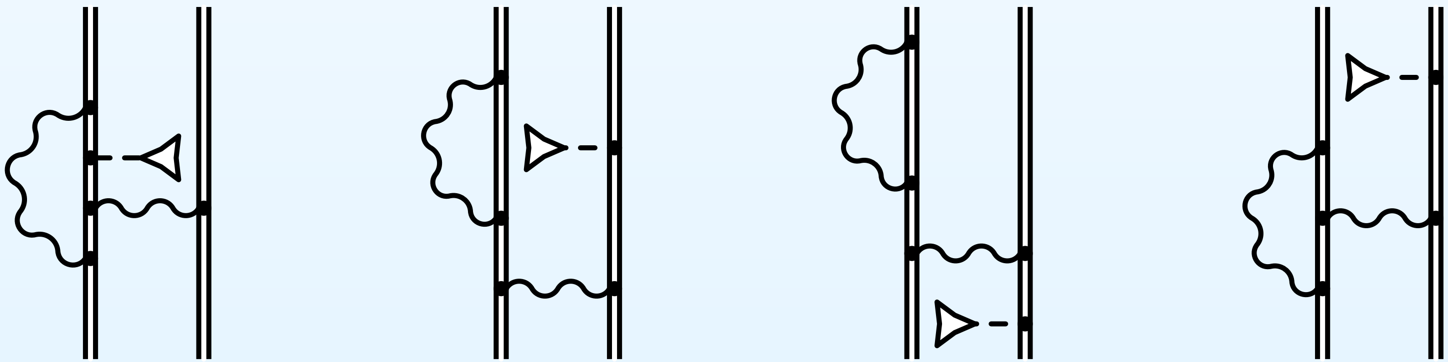
[R. N. Lee et al., PRA, 2005]

Many-electron one-loop QED corrections

Screened self-energy



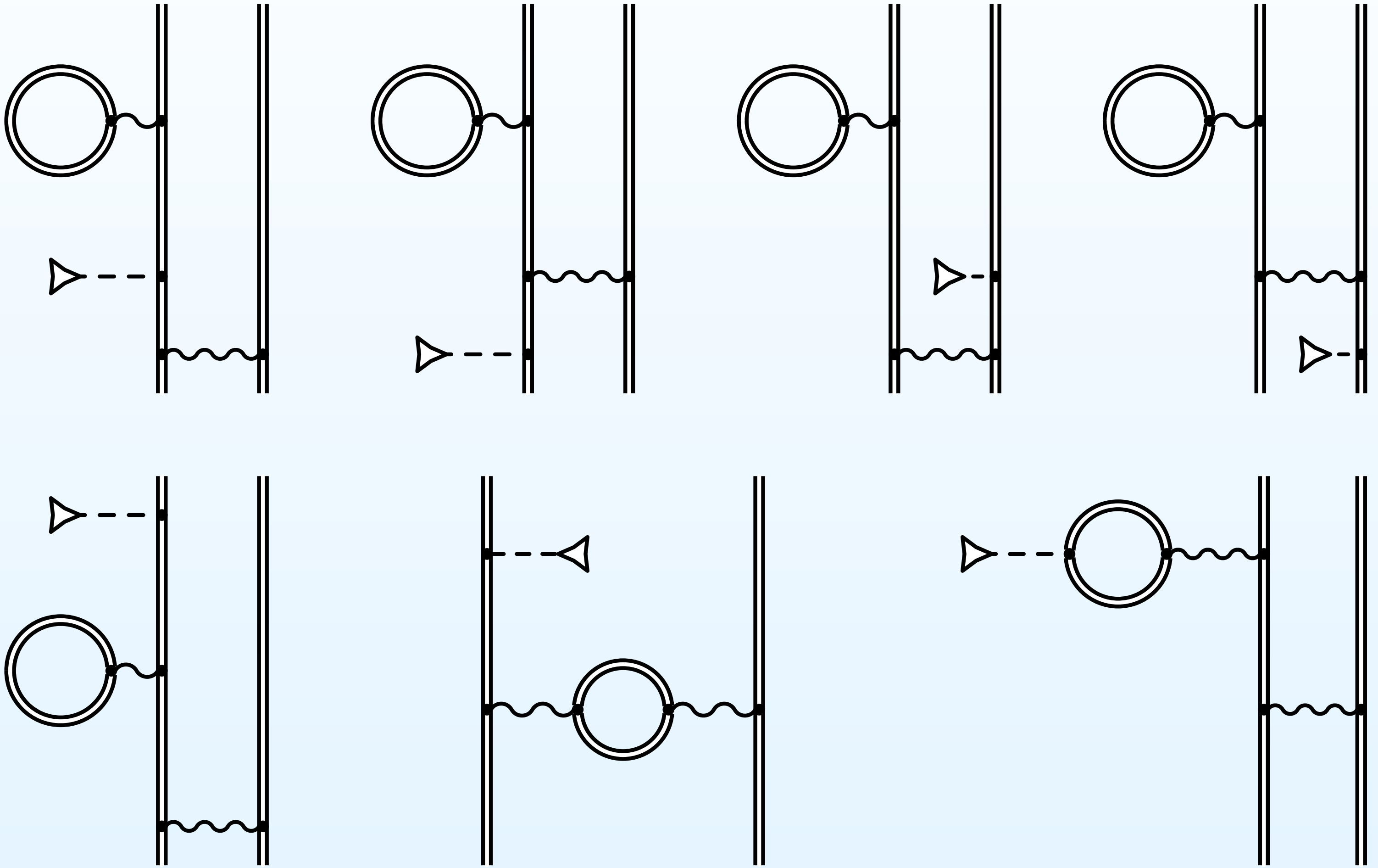
$(A1)$ $(A2)$ (B) $(C1)$ $(C2)$



(D) $(E1)$ $(E2)$ (F)

Many-electron one-loop QED corrections

Screened vacuum-polarization



Many-electron one-loop QED corrections

- Two-time Green function method
- Finite basis set: DKB B-splines
- Feynman and Coulomb gauges

$$\Delta g^{\mathrm{A,B,E}}[\mathrm{UV}] \sim \frac{i}{2\pi}\int \mathrm{d}\omega \sum_{n_1} \frac{\langle X n_1 | I(\omega) | n_1 Y\rangle}{(\varepsilon_a - \omega - \varepsilon_{\bar{n}_1})}$$

$$\Delta g^{\mathrm{C1}}[\mathrm{UV},\mathrm{IR}] \sim \frac{i}{2\pi}\int \mathrm{d}\omega \sum_{n_{1,2}} \frac{\langle X n_1 | I(\omega) | n_2 a\rangle \langle n_2 | T_0 | n_1\rangle}{(\varepsilon_a - \omega - \varepsilon_{\bar{n}_1})(\varepsilon_a - \omega - \varepsilon_{\bar{n}_2})}$$

$$\Delta g^{\mathrm{C2}}[\mathrm{UV},\mathrm{IR}] \sim \frac{i}{2\pi}\int \mathrm{d}\omega \sum_{n_{1,2}} \frac{\langle X n_1 | I(\omega) | n_2 a\rangle \langle n_2 b | I(\Delta) | n_1 b\rangle}{(\varepsilon_a - \omega - \varepsilon_{\bar{n}_1})(\varepsilon_a - \omega - \varepsilon_{\bar{n}_2})}$$

$$\Delta g^{\mathrm{D}}[\mathrm{IR}] \sim \frac{i}{2\pi}\int \mathrm{d}\omega \sum_{n_{1,2,3}} \frac{\langle a n_1 | I(\omega) | n_3 a\rangle \langle n_3 b | I(\Delta) | n_2 b\rangle \langle n_2 | T_0 | n_1\rangle}{(\varepsilon_a - \omega - \varepsilon_{\bar{n}_1})(\varepsilon_a - \omega - \varepsilon_{\bar{n}_2})(\varepsilon_a - \omega - \varepsilon_{\bar{n}_3})}$$

g factor of Li-like Pb

Dirac value (point nucleus)	1.932 002 904
Interelectronic interaction	0.002 140 7 (27)
QED, one-loop	0.002 411 7 (1)
QED, two-loop	-0.000 003 6 (5)
	-0.000 003 5 (12)
QED, screening	-0.000 001 8 (2)
Recoil	0.000 000 2 (3)
Nuclear size	0.000 078 6 (1)
Nuclear polarization	-0.000 000 04 (2)
	1.936 627 0 (30)
Total theory	1.936 628 7 (28)

[A. V. Volotka, D. A. Glazov, V. M. Shabaev, I. I. Tupitsyn, G. Plunien, PRL, 2009]

Conclusion and Outlook

⋆ Experimental and theoretical investigations of the bound-electron g factor in heavy highly charged ions will provide

$\longrightarrow$ an independent determination of the fine structure constant α

$\longrightarrow$ accurate tests of QED in strong Coulomb field

⋆ A significant step towards high theoretical accuracy:

$\longrightarrow$ screened self-energy diagrams

$\longrightarrow$ screened vacuum-polarization diagrams (Uehling approximation)

have been evaluated.

⋆ Next step is to evaluate:

$\longrightarrow$ two-photon exchange diagrams

$\longrightarrow$ screened vacuum-polarization diagrams (complete)