Higher-order QED contributions to the g factor of heavy ions

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

St. Petersburg State University
Institut für Theoretische Physik, TU Dresden

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- g factor of few-electron ions
- Determination of α
  - Free-electron v.s. bound-electron g factor
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High-Z few-electron ions

$\alpha = 1/137.036...$, Z – nuclear charge, $V_{\rm nuc}(r) = -\dfrac{\alpha Z}{r}$

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

$$\mathcal{E}[\mathrm{H}(1\mathrm{s})] = 10^{10}\mathrm{V/cm}$$
$$\mathcal{E}[\mathrm{Laser}] = 10^{12}\mathrm{V/cm}$$
$$\mathcal{E}[\mathrm{U}(1\mathrm{s})] = 10^{16}\mathrm{V/cm}$$

High-Z systems: $\alpha Z \sim 1 \longrightarrow$ no expansion in αZ — strong-field regime of QED

The most precise test — Lamb shift in Li-like uranium.

Theory: 280.71(10) eV *[Y.S. Kozhedub et al., PRA (2008)]*

Experiment: 280.645(15) eV *[P. Beiersdorfer et al., PRL (2005)]*

g factor of few-electron ions

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)]*

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

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

in progress: Si, Ar

planned: Pb, U

Determination of α: free-electron g factor

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

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

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

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

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

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

Determination of α: bound-electron g factor

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

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

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

$$\mathrm{Pb}\ \ (Z=82): \quad \delta g_{1s}^{\mathrm{exp}} = 0.7\times10^{-9} \rightarrow \frac{\delta\alpha}{\alpha} = 1.3\times10^{-9}$$

However there is a problem:

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

For $r \leq R_{\rm nuc}$ the binding energy in the Dirac equation can be neglected.
$\Rightarrow$ for $1s$ and $2s$ states:

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

Let us introduce the parameter ξ

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

and the specific difference g'

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

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

B-like ions

For high Z for $r \leq R_{\mathrm{nuc}}$ even the mc^2 in the Dirac equation can be neglected.
$\Rightarrow$ for $1s$ and $2p_{1/2}$ states:

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

Let us introduce the parameter ξ

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

and the specific difference g'

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

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

Moreover, $\mathrm{d}g'/\mathrm{d}\alpha$ is larger than for the Li-like ions.

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)]

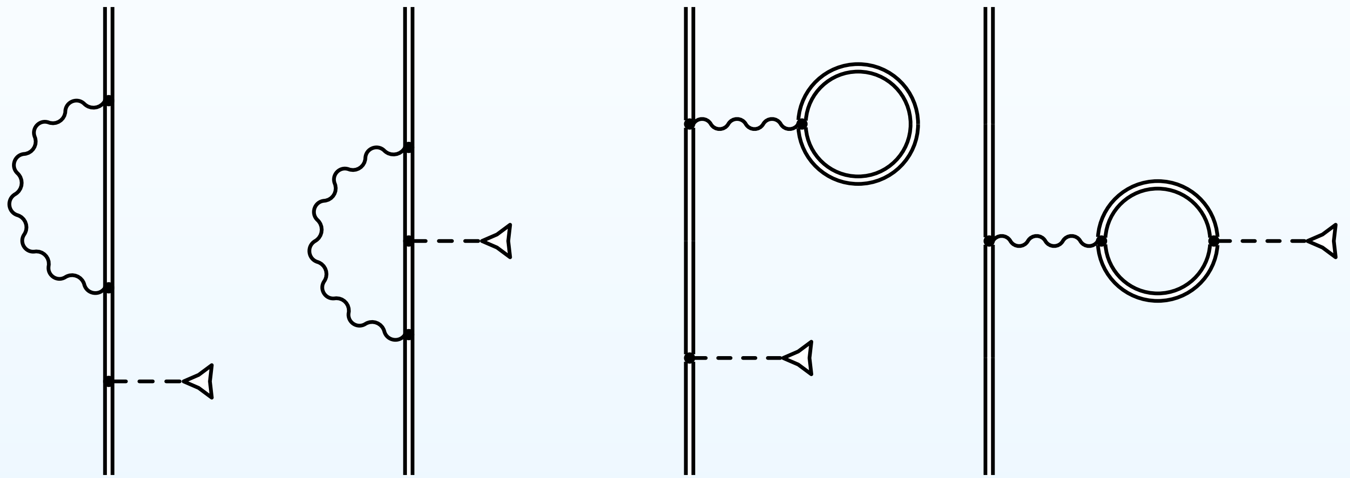
Theoretical status and recent developements

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

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

One-electron one-loop QED

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



$$\Delta g_{\rm QED} = \Delta g_{\rm SE} + \Delta g_{\rm VP}$$

Coulomb field:

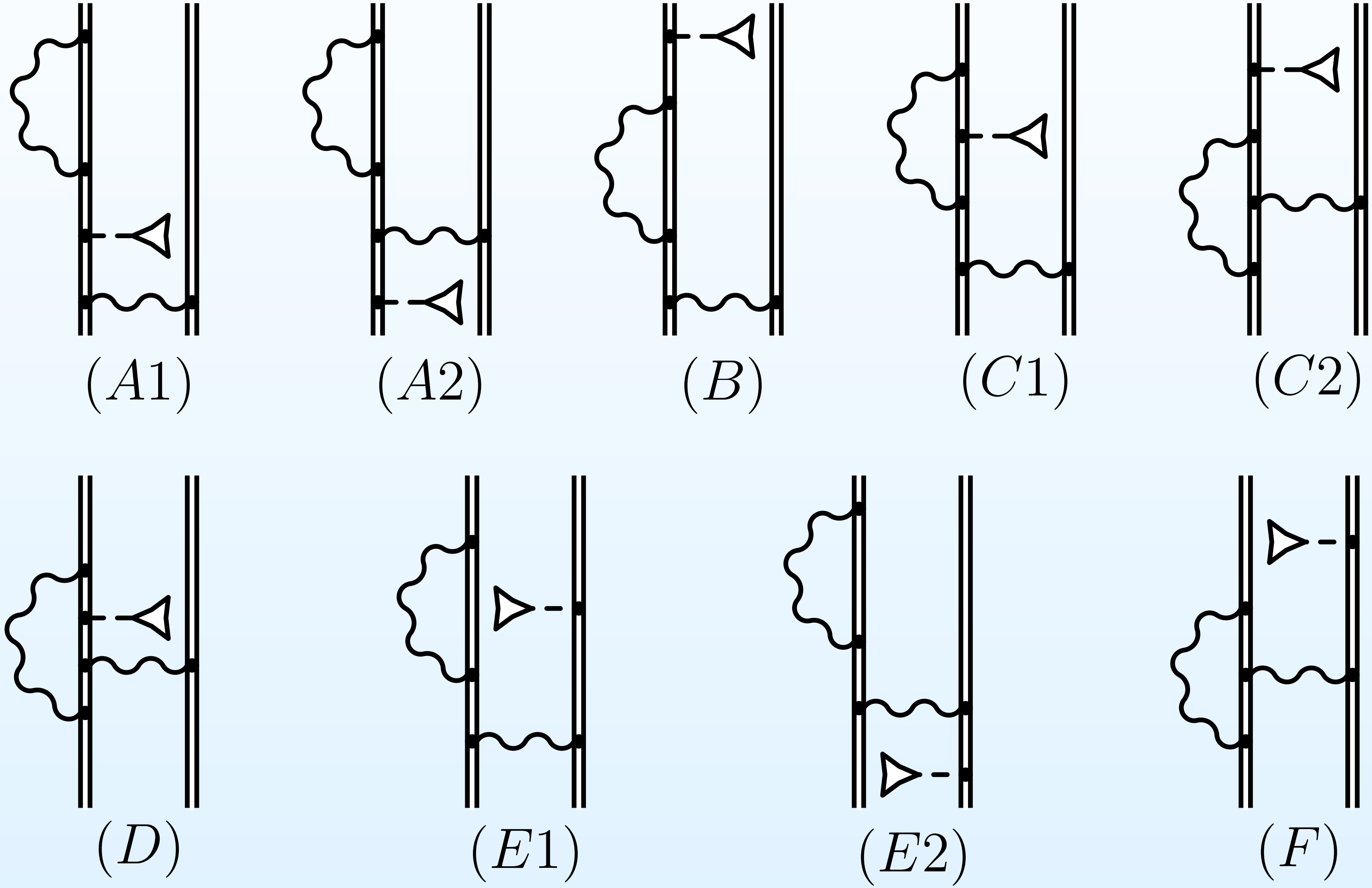
[V. A. Yerokhin et al., PRA (2004)], *[R. N. Lee et al., PRA (2005)]*

Effective screening potential:

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

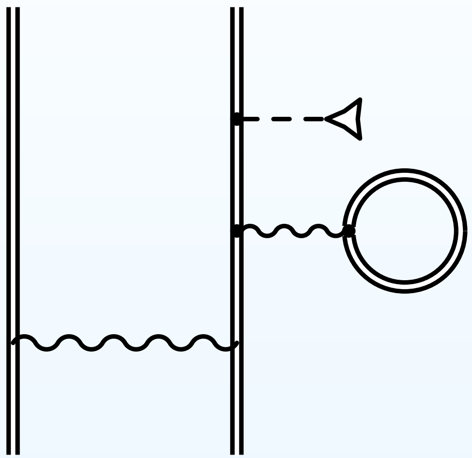
Many-electron one-loop QED

Screened self-energy

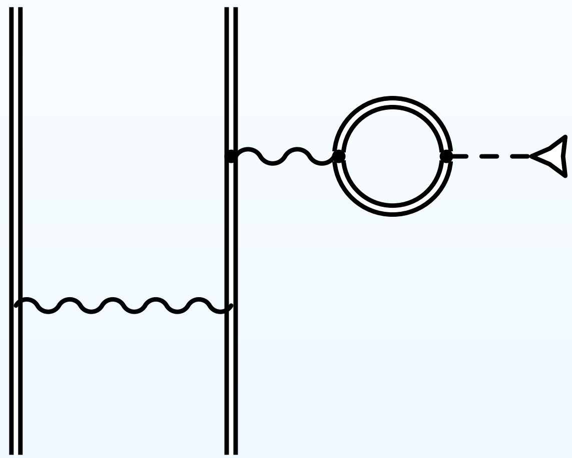


Many-electron one-loop QED

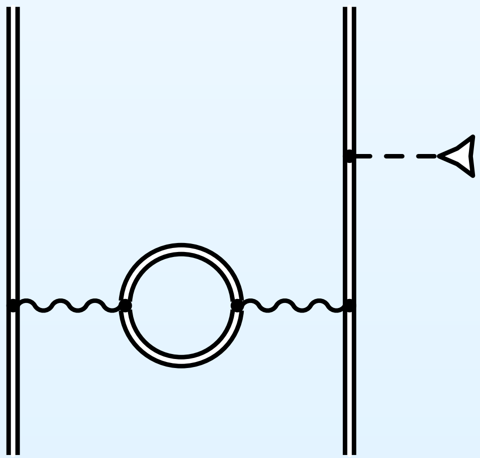
Screened vacuum-polarization



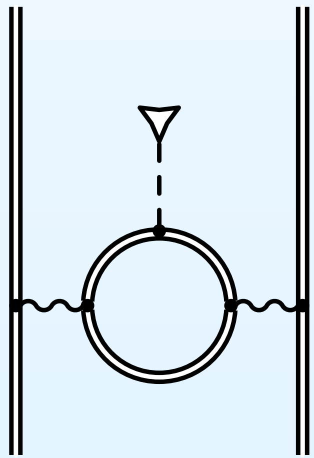
(A)



(B)



(C)

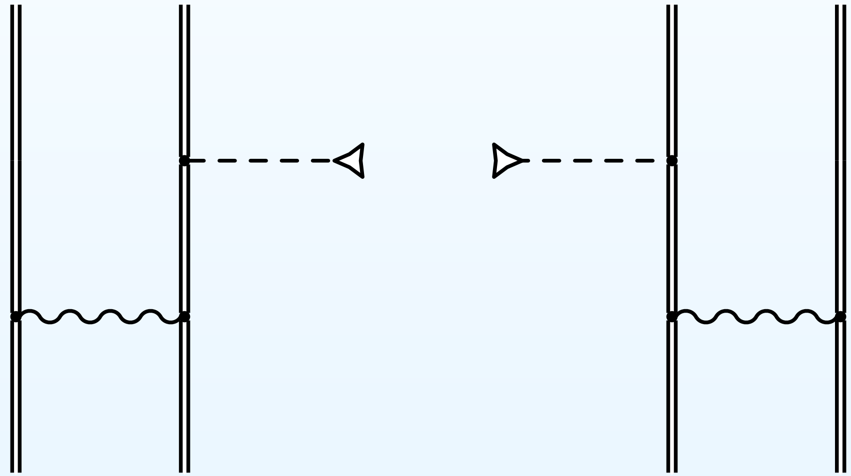


(D)

Interelectronic interaction

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

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



$1/Z^2$ and higher:

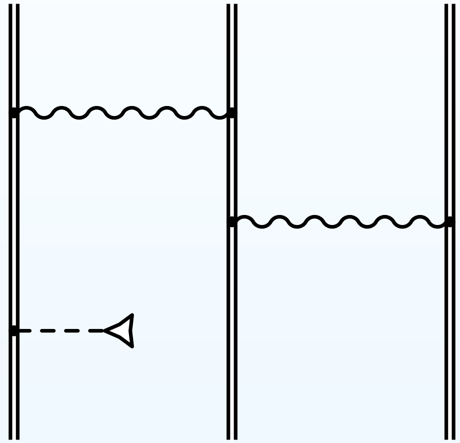
large-scale configuration-interaction Dirac-Fock-Sturm method

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

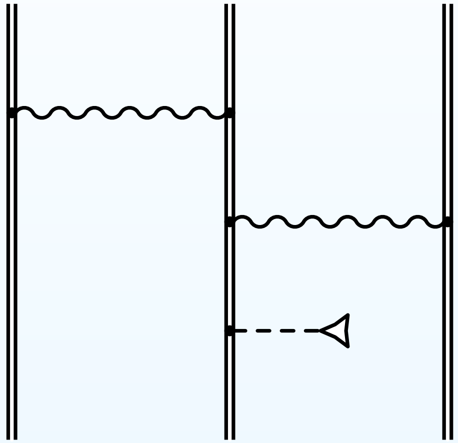
[V. M. Shabaev et al., PRA (2002)], [D. A. Glazov et al., PRA (2004)]

Two-photon exchange

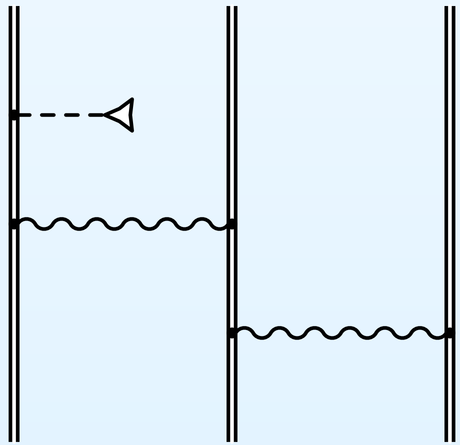
Three-electron diagrams



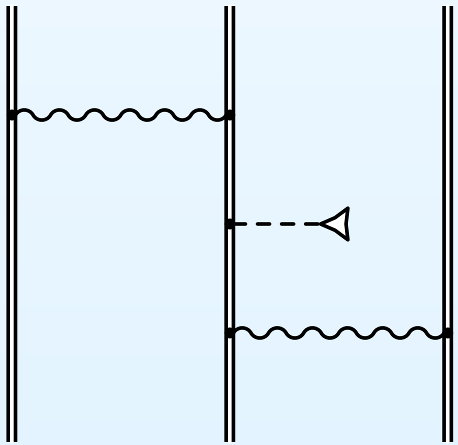
$(1L)$



$(2L)$



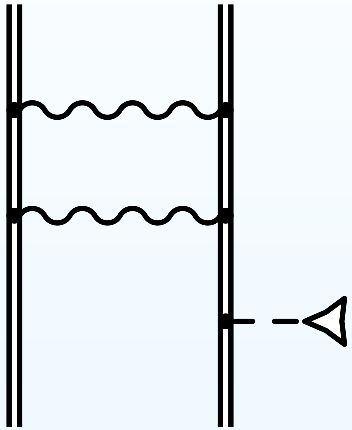
$(1R)$



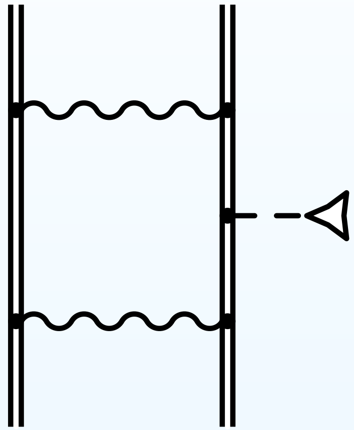
(S)

Two-photon exchange

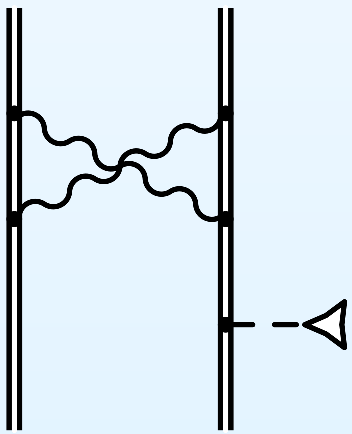
Two-electron diagrams



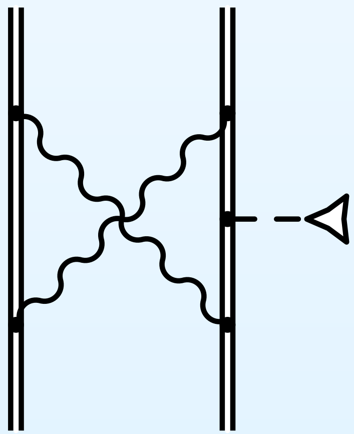
$(\text{ladder}-L)$



$(\text{ladder}-S)$



$(\text{cross}-L)$



$(\text{cross}-S)$

Evaluational procerdure

- Derivation of the general formulae: the two-time Green function method

$$\Delta g^{\mathrm{D}} = \frac{i}{2\pi} \int \mathrm{d}\omega \sum_{n_{1,2,3}} \frac{\langle a n_1 | I(\omega) | n_3 a \rangle \langle n_3 b | I(\Delta) | n_2 b \rangle \langle n_2 | T_0 | n_1 \rangle}{(\varepsilon_a - \omega - \varepsilon_{\overline{n_1}})(\varepsilon_a - \omega - \varepsilon_{\overline{n_2}})(\varepsilon_a - \omega - \varepsilon_{\overline{n_3}})}$$

- Ultraviolet divergencies: potential expansion
  - 0,1-potential terms: momentum space
  - many-potential term: coordinate space
- Infrared divergencies:
  - proof the cancellation analytically
  - evaluate the sum numerically
- Numerical procedure:
  - partial-wave expansion
  - finite basis set: DKB-splines
- Feynman and Coulomb gauges

g factor of Li-like Pb

Dirac value (point nucleus)	1.932 002 904
e^-–e^- interaction, $1/Z$	0.002 148 29
e^-–e^- interaction, $1/Z^{2+}$	0.000 007 6 (27)
QED, one-loop	0.002 411 7 (1)
QED, two-loop	-0.000 003 6 (5)
QED, screening	-0.000 001 8 (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 7 (28)

g factor of Li-like U

Dirac value (point nucleus)	1.910 722 624
e^-–e^- interaction, $1/Z$	0.002 509 84
e^-–e^- interaction, $1/Z^{2+}$	0.000 008 5 (38)
QED, one-loop	0.002 446 3 (2)
QED, two-loop	-0.000 003 6 (8)
QED, screening	-0.000 001 7 (1)
Recoil	0.000 000 3 (7)
Nuclear size	0.000 241 3 (4)
Nuclear polarization	-0.000 000 2 7 (14)
Total theory	1.915 904 9 (40)

Conclusion and Outlook

$\star$ Experimental and theoretical investigations of the bound-electron g factor in highly charged ions will provide
$\longrightarrow$ accurate tests of QED in strong Coulomb field
$\longrightarrow$ an independent determination of the fine structure constant α

$\star$ A significant step towards high theoretical accuracy:
$\longrightarrow$ two-electron self-energy
$\longrightarrow$ two-electron vacuum-polarization (partly)
$\longrightarrow$ two-photon exchange

$\star$ Next steps are:
$\longrightarrow$ higher-order interelectronic interaction
$\longrightarrow$ two-electron vacuum polarization (WK-ml, D)
$\longrightarrow$ lower nuclear charge Z
$\longrightarrow$ B-like ions

thank you for your attention!