Precision theory of the bound-electron g factor

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Matter To The Deepest

Podlesice, Poland
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Collaboration

- **Theory, MPIK:**
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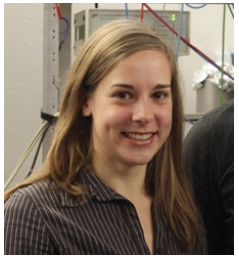
- **Theory, St. Petersburg, Russia:**
  V. A. Yerokhin, I. I. Tupitsyn, E. Berseneva

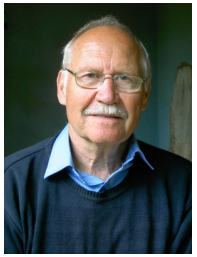


- **Theory, Warsaw and Poznan, Poland:**
  K. Pachucki, M. Puchalski


- **Penning trap experiments, MPIK/Mainz University/GSI:**
  S. Sturm, F. Köhler-Langes,
  A. Kracke (Wagner), B. Schabinger,
  G. Werth, W. Quint, K. Blaum







The g factor of a free electron

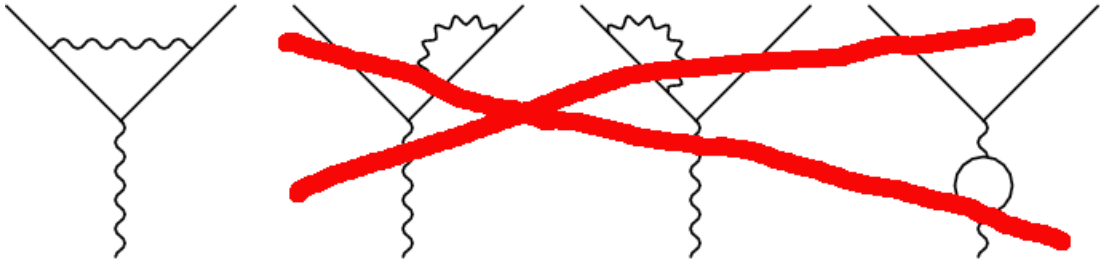
Energy shift due to interaction with an external magnetic field:

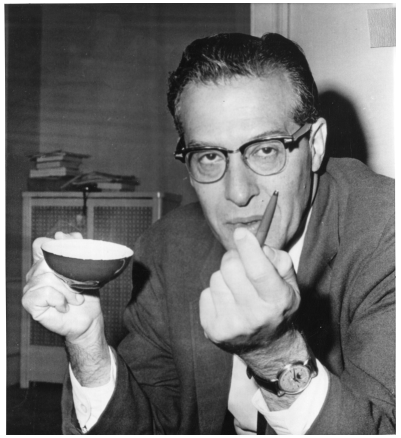
$$\delta E = \left\langle -\vec{\mu} \cdot \vec{B} \right\rangle, \text{with the magnetic moment} \quad \vec{\mu} = g \frac{q}{2m} \vec{s}$$

For a free electron:

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

- One-loop correction: only the vertex correction contributes
- Vertex correction: $\frac{\alpha}{2\pi}$, calculated by J. Schwinger
  Phys. Rev. **73**, 416 (1948)

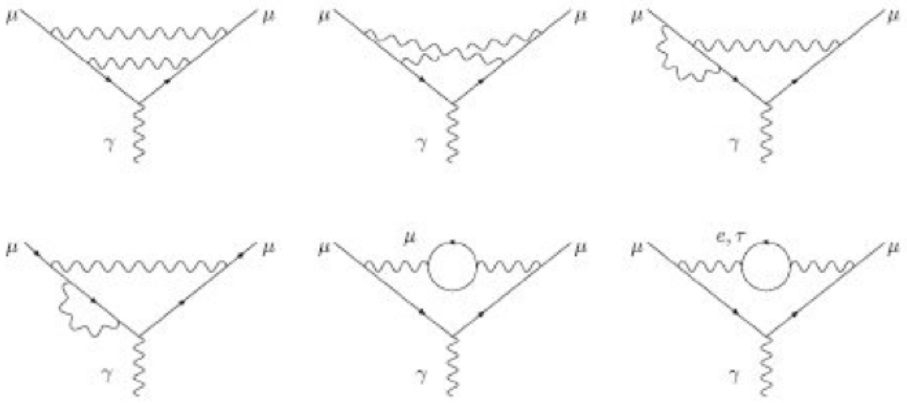




Dirac and Feynman at the Relativity conference, Jabłonna Palace, 1962

$$2 \quad + \quad \frac{\alpha}{\pi}$$

Two-loop diagrams:



A. Peterman, Helv. Phys. Act **30**, 407 (1957);
C. M. Sommerfield, Ann. Phys. **5**, 26 (1958)

Three$^+$-loop diagrams:

S. Laporta, E. Remiddi, Phys. Lett. B **379**, 283 (1996)

T. Aoyama, M. Hayakawa, T. Kinoshita, M. Nio, Phys. Rev. Lett. **109**, 111807 (2012)

S. Laporta, arXiv:1704.06996 (2017) (1100 digits of the 4-loop coefficient!)

Current best experimental value:

$$g_{\text{exp}} = 2.002\,319\,304\,361(6)$$

The CODATA value of the **fine-structure constant** is largely determined by g_{exp} and corresponding multi-loop free-electron QED calculations

D. Hanneke, S. Fogwell, and G. Gabrielse, Phys. Rev. Lett. **100**, 120801 (2008)

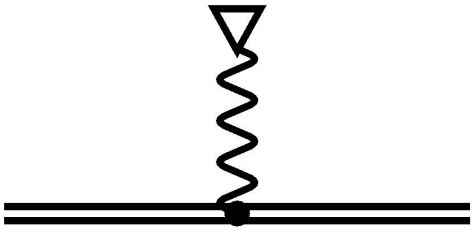
The Dirac value of the bound-electron g factor

System described by the Dirac Hamiltonian with a scalar potential $V(\vec{r})$

$$H = \vec{\alpha} \cdot \vec{p} + \beta m + V(\vec{r}) - e\vec{\alpha} \cdot \vec{A}$$

and the perturbing field $\vec{A} = \frac{1}{2}\left(\vec{B} \times \vec{r}\right)$. The magnetic correction to the energy (Zeeman shift):

$$\delta E = -e \left\langle \vec{\alpha} \cdot \vec{A} \right\rangle .$$



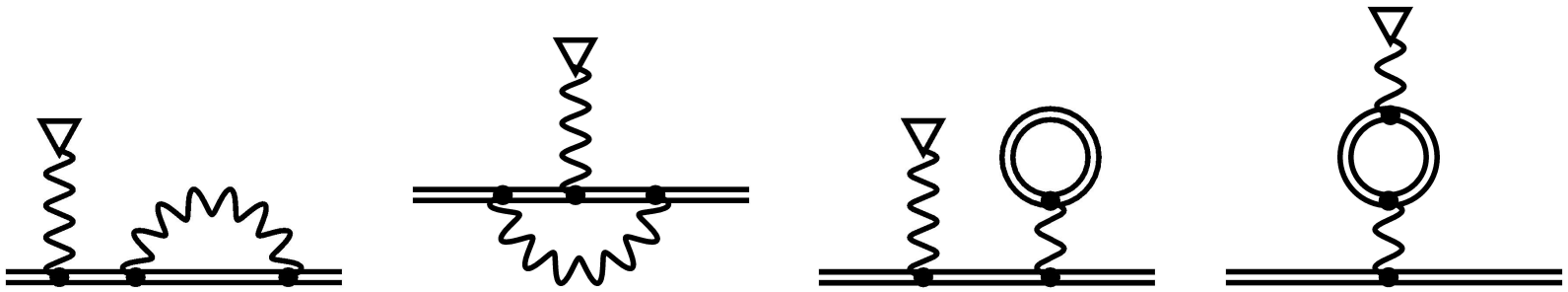
In case of the Coulomb potential, the Dirac g-factor for the $1s$ state (G. Breit, 1928):

$$g_{\mathrm{D}} = \frac{2}{3}\left(1 + 2\sqrt{1 - (Z\alpha)^2}\right) = 2 - \frac{2}{3}(Z\alpha)^2 - \frac{1}{6}(Z\alpha)^4 + \dots .$$

A number of corrections contribute to $g_{\rm th}$:

$$g_{\rm th} = g_{\rm D} + \delta g_{\rm 1L} + \delta g_{\rm 2L} + \delta g_{\rm FS} + \delta g_{\rm rec} + \delta g_{\rm ND} + \delta g_{\rm NP}\,,$$

$\delta g_{\rm 1L}$ – one-loop QED: self-energy (SE) and vacuum polarization (VP),
$\delta g_{\rm 2L}$ – two-loop QED: SE-SE, VP-VP, SE-VP,
$\delta g_{\rm FS}$ – nuclear finite-size,
$\delta g_{\rm rec}$ – recoil,
$\delta g_{\rm ND}$ – nuclear deformation,
$\delta g_{\rm NP}$ – nuclear polarizability,
...



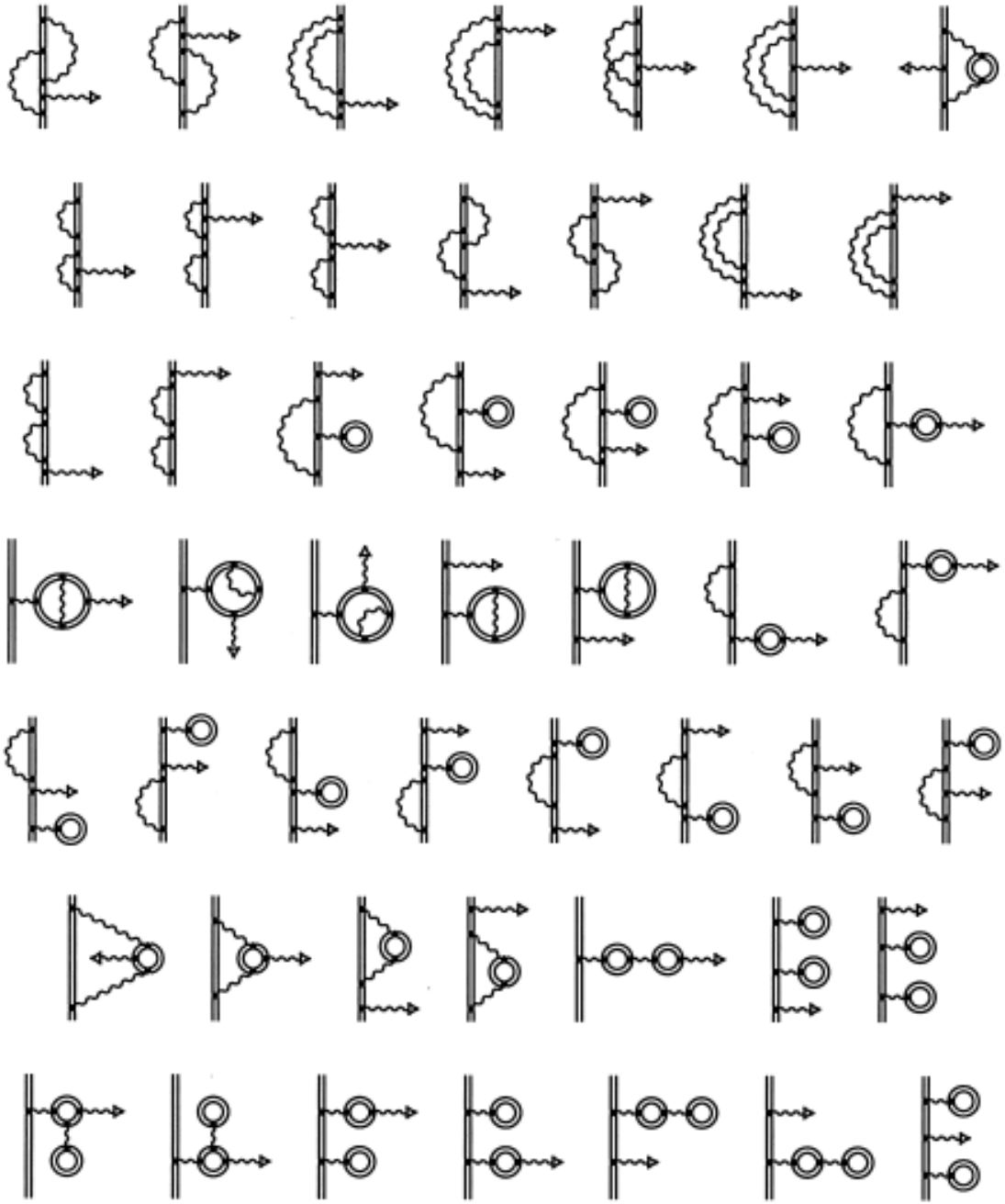
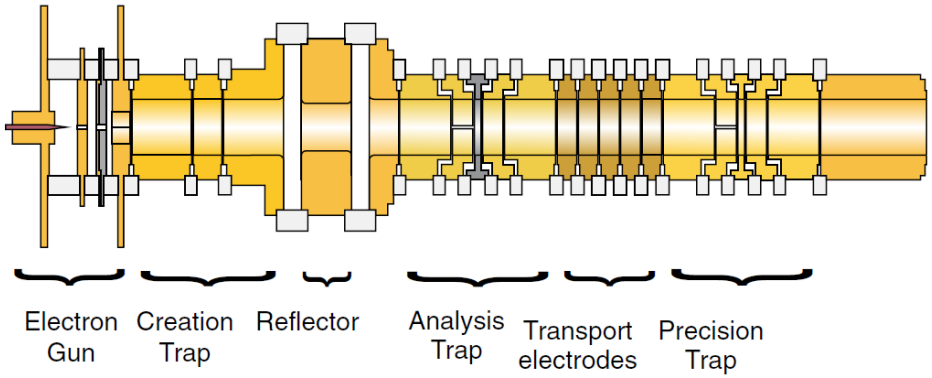
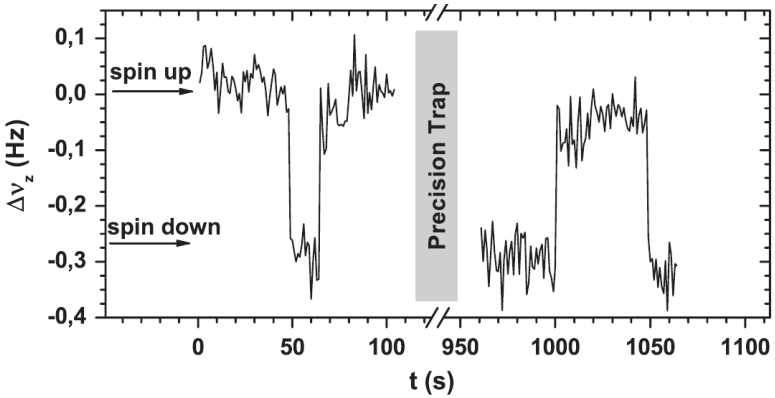


Figure from T. Beier, 2002

Penning trap measurement of the g factor





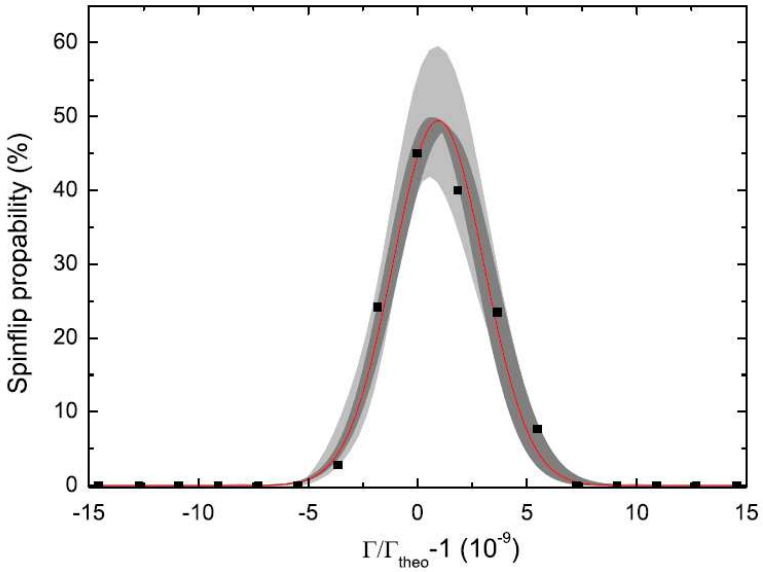
Larmor frequency:

$$\nu_{\mathrm{L}} = g\mu_B B \frac{1}{2\pi} = g\frac{e}{4\pi m_e} B\,,$$

Cyclotron frequency:

$$\nu_{\mathrm{c}} = \frac{qB}{2\pi M}\,,$$

$$\rightarrow \quad g_{\mathrm{exp}} = 2\frac{\nu_{\mathrm{L}}}{\nu_{\mathrm{c}}}\frac{m_e}{M}\frac{q}{e}$$



Results for $^{28}Si^{13+}$ (Z=14)

Theory			
Dirac value		1.993 023 571 6	Breit 1928
Finite nuclear size		0.000 000 020 5	
One-loop QED	$(Z\alpha)^0$	0.002 322 819 5	$\frac{\alpha}{\pi}$, Schwinger 1948
	$(Z\alpha)^2$	0.000 004 040 7	$\frac{\alpha}{\pi}\frac{(Z\alpha)^2}{6}$, Grotch 1970
	$(Z\alpha)^4$	0.000 001 244 6	Pachucki *et al.* 2004
	h.o. SE	0.000 000 542 8(3)	Yerokhin, Indelicato, Shabaev 2004, & Jentschura
	VP WK	0.000 000 032 6	Beier 2000
	VP magn.	0.000 000 002 5	Lee, Milstein, Terekhov, Karshenboim 2005
Two-loop QED	$(Z\alpha)^0$	-0.000 003 515 1	$\propto (\frac{\alpha}{\pi})^{2+}$, Sommerfield 1958, Kinoshita et al.
	$(Z\alpha)^2$	-0.000 000 006 1	Grotch 1970
	$(Z\alpha)^4$	-0.000 000 001 3	Pachucki, Czarnecki, Jentschura, Yerokhin 2005
	h.o.	0.000 000 000 0(17)	
Recoil	m/M	0.000 000 206 1(1)	Shabaev, Yerokhin 2002
	rad-rec	-0.000 000 000 2	Grotch 1970
	$(m/M)^{2+}$	-0.000 000 000 1	Pachucki 2008
Total theory		1.995 348 958 0(17)	
Experiment (2011)		1.995 348 958 7(5)(3)(8)	(stat)(syst)(m_e)

Extraction of the nuclear radius: $R_{\rm rms}$ =3.18(15) fm (proof-of-the-principle determination)

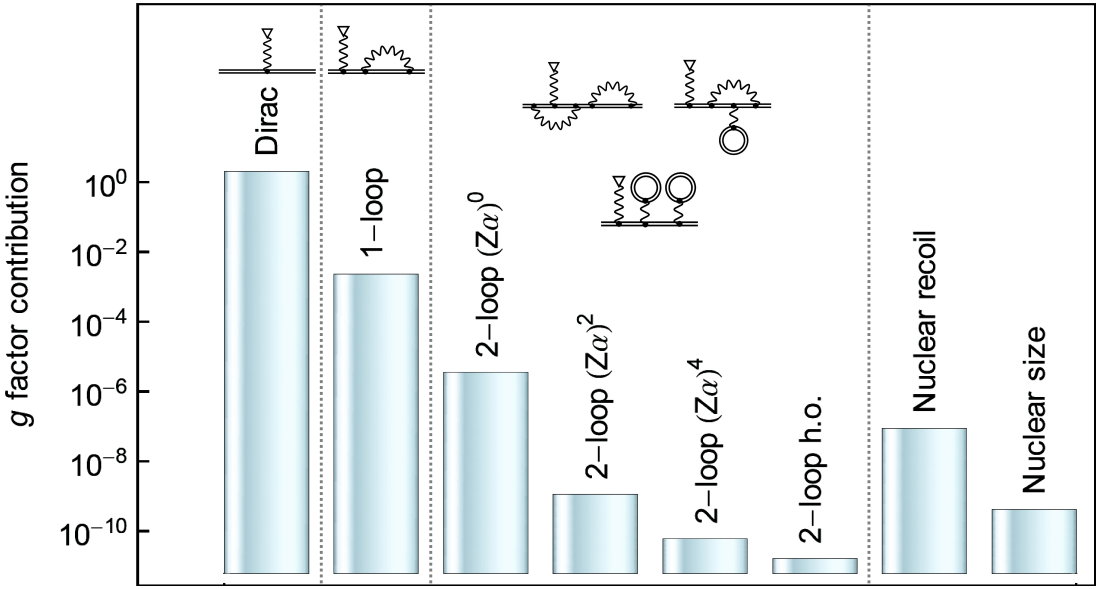
- S. Sturm, A. Wagner, B. Schabinger, J. Zatorski, Z. H., W. Quint, G. Werth, C. H. Keitel, K. Blaum, Phys. Rev. Lett. **107**, 023002 (2011)
- S. Sturm, A. Wagner, M. Kretzschmar *et al.*, Phys. Rev. A **87**, 030501(R) (2013)

High-precision determination of the electron mass

The mass of the electron can be expressed by the mass and charge of the $^{12}C^{5+}$ ion, the experimentally measured cyclotron and Larmor frequencies, and the theoretical g-factor as

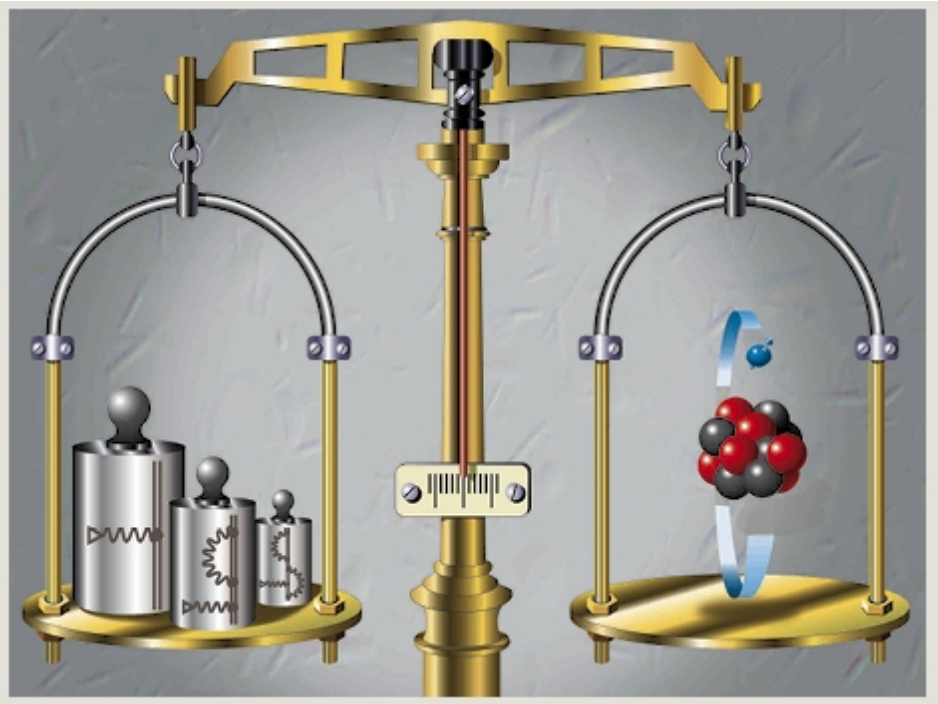
$$m_e = \frac{g}{2}\frac{e}{Q}\frac{\nu_c}{\nu_L}m_{\text{ion}}$$

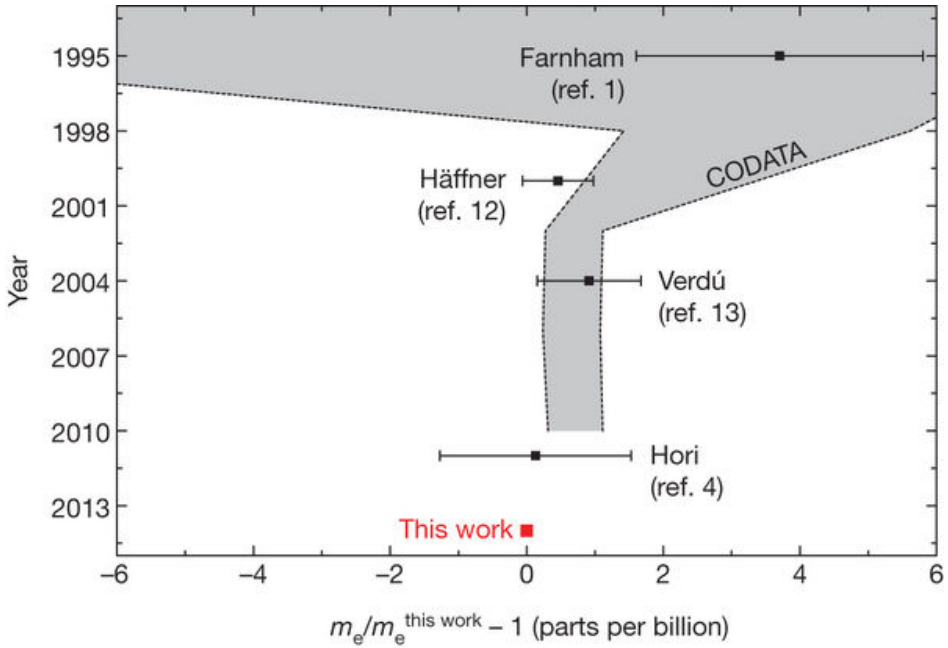
- $e/Q = 1/6$;
- m_{ion} is known very well ($m_{^{12}\text{C atom}} \equiv 12$ u);
- ν_c/ν_L is measured very precisely;
- the g-factor is taken from theory



The resulting value $m_e = 0.000\,548\,579\,909\,069\,4(128)_{\text{stat}}(86)_{\text{sys}}(13)_{\text{theo}}$ u surpasses the earlier CODATA value by more than an order of magnitude and largely defines the new CODATA value

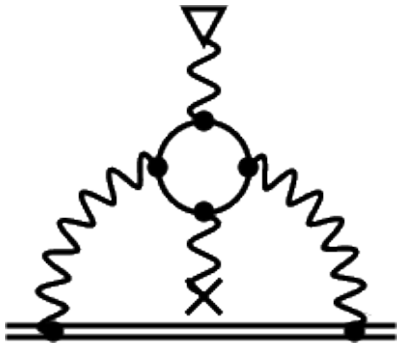
- S. Sturm, F. Köhler, J. Zatorski, A. Wagner, Z. H., G. Werth, W. Quint, C. H. Keitel, K. Blaum, Nature **506**, 467 (2014)
- F. Köhler, S. Sturm, A. Kracke, G. Werth, W. Quint, and K. Blaum, J. Phys. B **48**, 144032 (2015)




Year
1995
1998
2001
2004
2007
2010
2013
Farnham
(ref. 1)
Häffner
(ref. 12)
CODATA
Verdú
(ref. 13)
Hori
(ref. 4)
This work
−6
−4
−2
0
2
4
6
$m_e/m_e^{\text{this work}} - 1$ (parts per billion)

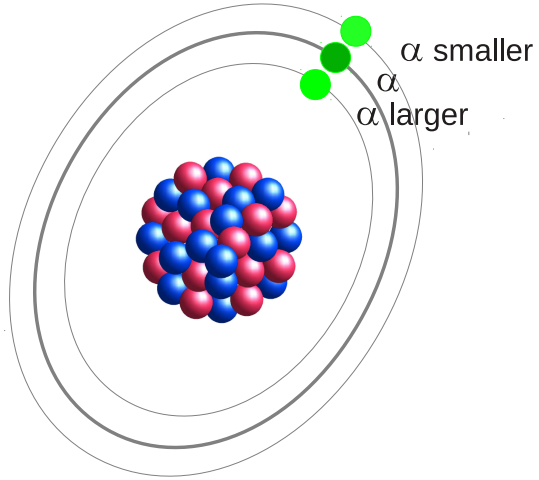
Contribution	$^4He^+$	$^{12}C^{5+}$	Ref.
(Zero- and one-loop QED ...)			
Two-loop QED			
$(Z\alpha)^0$	-0.000 003 544 604 49	-0.000 003 544 604 5	Peterman 1957, Sommerfield 1958
$(Z\alpha)^2$	-0.000 000 000 125 84	-0.000 000 001 132 5	Grotch 1970
$(Z\alpha)^4$ (w/o LBL)	0.000 000 000 002 41	0.000 000 000 060 1	Pachucki, Czarnecki, Yerokhin, Jentschura 2005
LBL at $(Z\alpha)^4$	-0.000 000 000 000 39	-0.000 000 000 0**31 5**	Czarnecki, Szafron 2016
$(Z\alpha)^{5+}$ S(VP)E	0.000 000 000 000 00	0.000 000 000 000 0(1)	Yerokhin, Z. H. 2013
$(Z\alpha)^{5+}$ SEVP	0.000 000 000 000 03	0.000 000 000 006 9(3)	ditto
$(Z\alpha)^{5+}$ VPVP	0.000 000 000 000 03	0.000 000 000 005 5	ditto, Jentschura 2009
$(Z\alpha)^{5+}$ SESE (estimate)	0.000 000 000 000 00(2)	-0.000 000 000 001 2(33)	
$\geq$ Three-loop QED			
$(Z\alpha)^0$	0.000 000 029 497 95	0.000 000 029 497 9	Laporta, Remiddi 1996, Aoyama *et al.* 2012
$(Z\alpha)^2$	0.000 000 000 001 05	0.000 000 000 009 4	Grotch 1970
(Recoil ...)			
Weak interaction at $(Z\alpha)^0$	0.000 000 000 000 06	0.000 000 000 000 1	Czarnecki, Krause, Marciano 1996
Hadronic effects at $(Z\alpha)^0$	0.000 000 000 003 47	0.000 000 000 003 5	Nomura 2013, Kurz 2014, Prades 2010
Total w/o SESE $(Z\alpha)^5$	2.002 177 406 711 68(87)	2.001 041 590 166 3(39)	
Total w/ SESE $(Z\alpha)^5$ from exp.	2.002 177 406 711 68(87)	2.001 041 590 165 2(51)	

- The inclusion of the virtual light-by-light scattering (LBL) contribution $\sim \alpha^2(Z\alpha)^4$ slightly changes m_e by +0.3 σ $\Rightarrow$ see the next talk by **Robert Szafron** Phys. Rev. A **94**, 060501(R) (2016)
- He^+ might be used for a cross-check and improvement of m_e



J. Zatorski, B. Sikora, S. G. Karshenboim, S. Sturm, F. Köhler-Langes, K. Blaum, C. H. Keitel, Z. H., Phys. Rev. A **96**, 012502 (2017).

Possible determination of the fine-structure constant from the g-factor

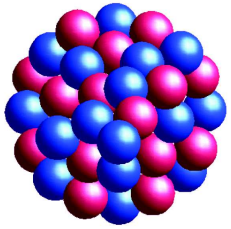


- In atoms/ions: Binding energies, wave functions and thus all properties depend on α
- Accurately determine the value α from atomic properties
  e.g. from the bound-electron g-factor – can be measured to very high accuracy
- Leading (Dirac) g-factor:
  $g_{\mathrm{D}} = {}^{2}/_{3}\left(1 + 2\sqrt{1-(Z\alpha)^2}\right)$

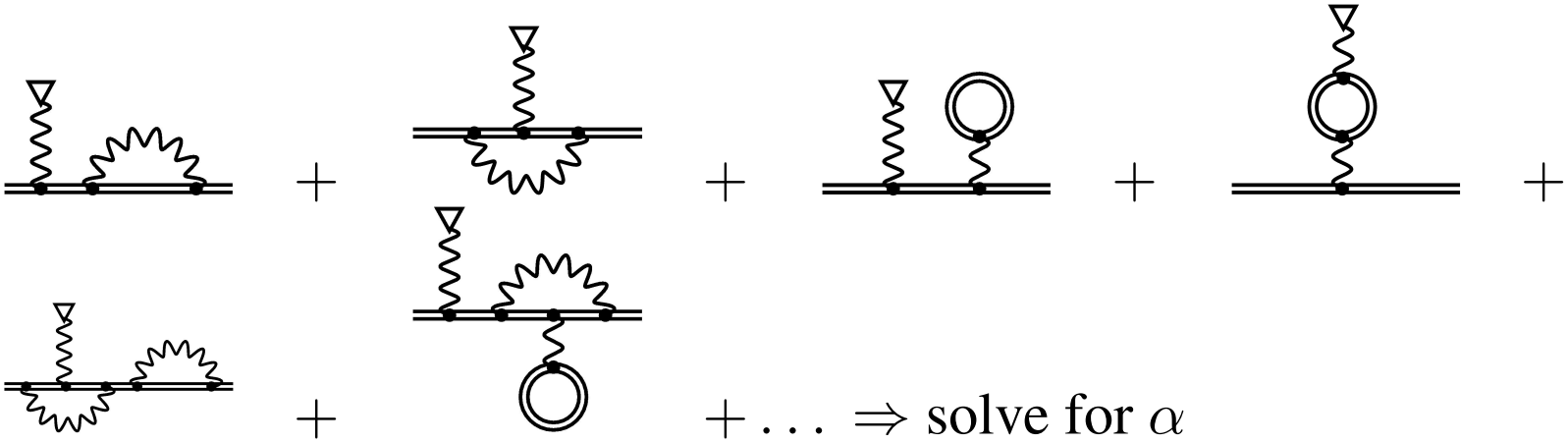
Determining α from the g-factor

Principle of determining α:

$$g_{\text{exp}} \stackrel{!}{=} g_{\text{theo}} = {}^{2}\!/_{3}\left(1 + 2\sqrt{1-(Z\alpha)^2}\right) \quad +$$



$+$



$+ \ldots \Rightarrow$ solve for α

- **Different physics** to determine α than in the case of the *free-electron* g-factor: dominant dependence not from a radiative correction (α/π), but from the binding ($Z\alpha$)
- **Enhanced sensitivity** as compared to the *free-electron* g-factor

- **Problem:** nuclear parameters (e.g. $\langle r^2 \rangle$) are not known accurately
- **Solution:** weighted difference of H- and Li-like ions (same Z):

$$\delta_\Xi g = g(2s) - \Xi g(1s)\,,$$

with the weight Ξ theoretically chosen to suppress nuclear size effects

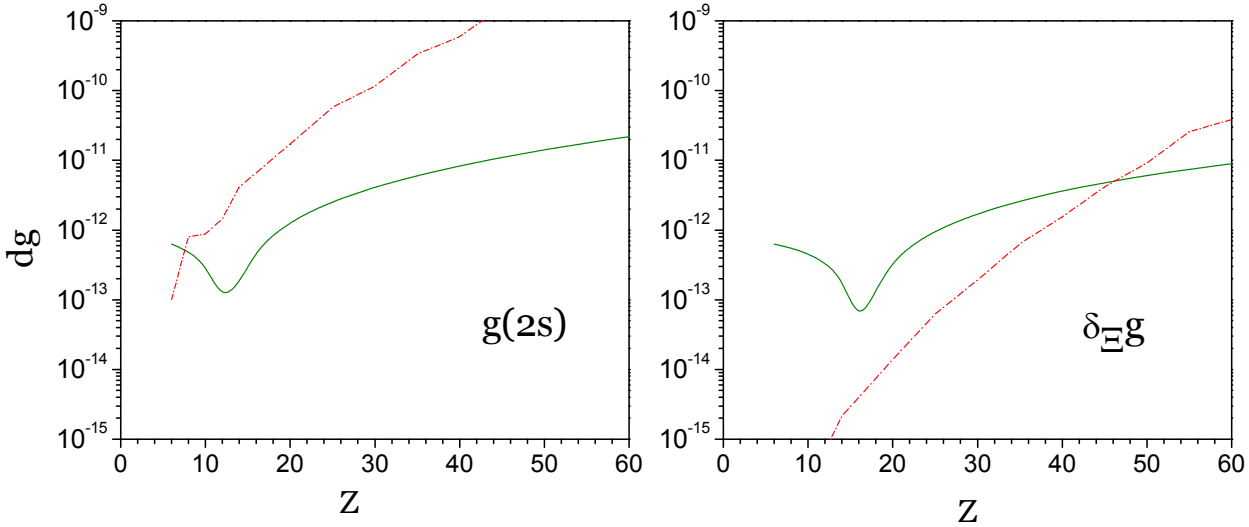
- Simplest approximation: $\Xi = \frac{1}{8} = 0.125$ – because: $|\psi_{ns}(r=0)|^2 \propto \frac{1}{n^3}$
- Accurate formula (incl. relativity, QED and e^-– e^- interaction:

$$\Xi = 2^{-2\gamma-1}\left[1 + \frac{3}{16}(Z\alpha)^2\right]\left(1 - \frac{2851}{1000}\frac{1}{Z} + \frac{107}{100}\frac{1}{Z^2}\right)\,,$$

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

error due to $\delta\langle r^2\rangle$ + distr. $\longrightarrow$

error due to present $\delta\alpha$ $\longrightarrow$



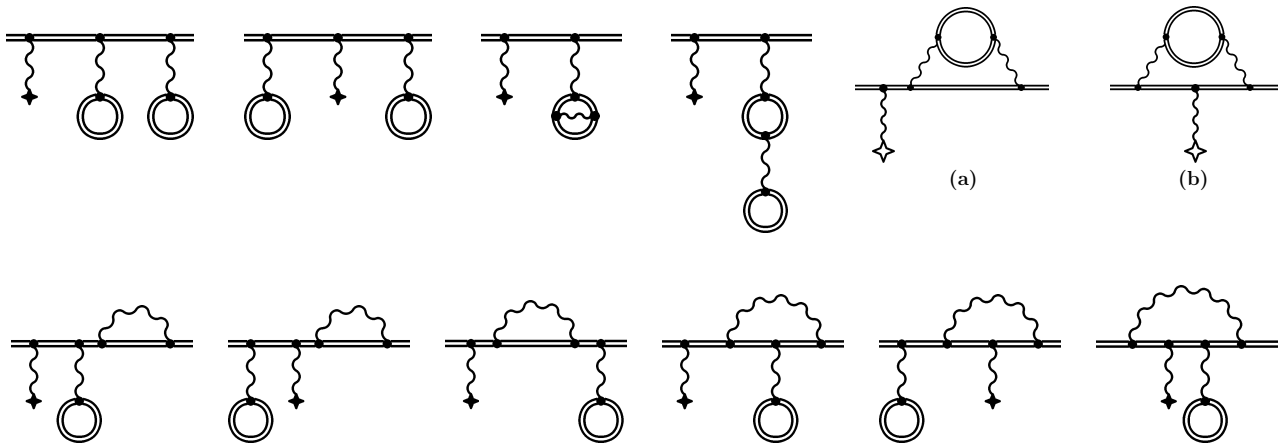
$\Rightarrow$ α can be significantly improved in principle

Earlier idea: weighted difference of **heavy** H- and B-like ions
V. M. Shabaev, D. A. Glazov, N. S. Oreshkina *et al.*, Phys. Rev. Lett. **96**, 253002 (2006)

- V. A. Yerokhin, E. Berseneva, Z. H., I. I. Tupitsyn, C. H. Keitel, Phys. Rev. Lett. **116**, 100801 (2016); Phys. Rev. A **94**, 022502 (2016)
- V. A. Yerokhin, C. H. Keitel, Z. H., J. Phys. B **46**, 245002 (2013)

α determination – to do list

- **improve the experiment...:** e.g. the new **ALPHATRAP** Penning trap setup
- **improve the theory:** I. H-like ions
  done: two-loop QED with one or two VP loops, non-perturbative in $Z\alpha$ (in the Uehling approximation):



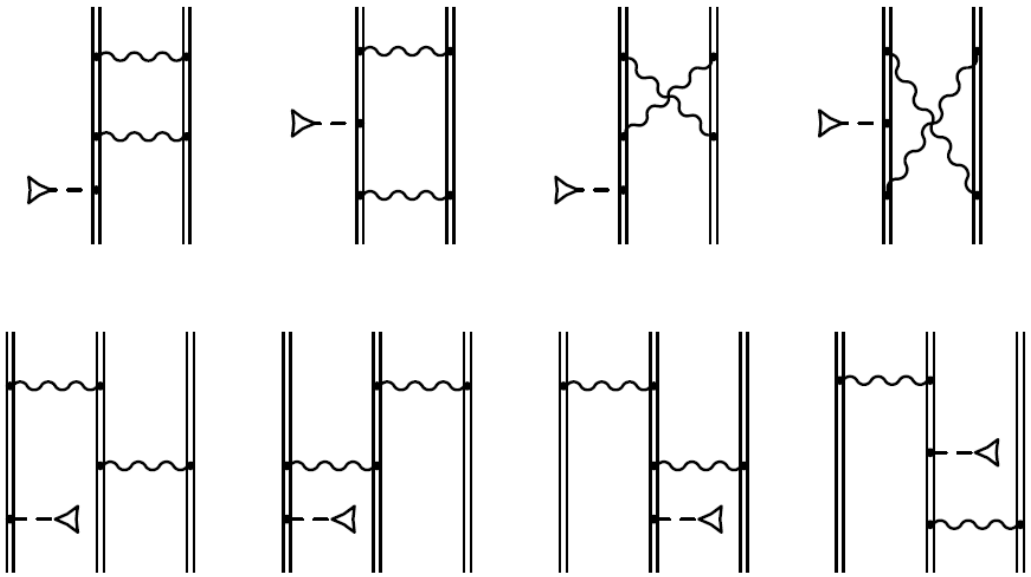
- V. A. Yerokhin, Z. H., Phys. Rev. A **88**, 042502 (2013)

One-loop self-energy

- non-perturbative in $Z\alpha$ evaluation with higher numerical accuracy – *two-digit improvement* for light ions
  V. A. Yerokhin, Z. H., Phys. Rev. A **95**, 060501(R) (2017)
- term of order $\alpha(Z\alpha)^5$ calculated analytically: K. Pachucki, M. Puchalski, Phys. Rev. A, accepted (2017); arXiv:1707.08518

α determination – to do list

- **improve the theory:** II. e^-e^- interaction in Li-like ions
  done: one- and two-photon exchange, non-perturbative in $Z\alpha$:



& extended with $\propto 1/Z^{3+}$ terms from a large-scale relativistic configuration interaction calculation

- A. Wagner, S. Sturm, F. Köhler, D. A. Glazov, A. V. Volotka, G. Plunien, W. Quint, G. Werth, V. M. Shabaev, K. Blaum Phys. Rev. Lett. **110**, 033003 (2013)
- A. V. Volotka, D. A. Glazov, V. M. Shabaev, I. I. Tupitsyn, G. Plunien, Phys. Rev. Lett. **103**, 033005 (2009)

α determination – to do list

However, $1/Z$ expansion – is not the most effective one at low Z

- NRQED: nonrelativistic, explicitly correlated, highly accurate wave functions; relativistic and QED effects calculated by expansion in $Z\alpha$
- Matching the two theories:
  - From $Z\alpha$ expansion: higher-order terms in $1/Z$
  - From $1/Z$ expansion: higher-order terms in $Z\alpha$

Related earlier NRQED calculations:

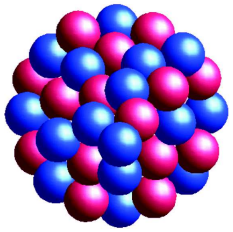
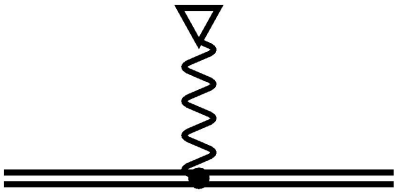
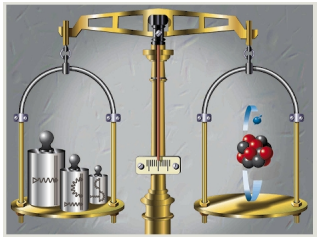
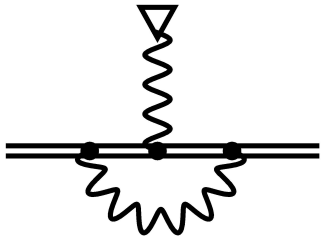
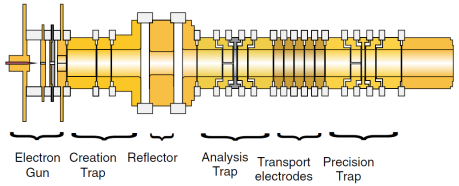
- Z.-C. Yan, Phys. Rev. Lett. **86**, 5683 (2001); J. Phys. B **35**, 1885 (2002)
- M. Puchalski, K. Pachucki, Phys. Rev. A 79, 032510 (2009); Phys. Rev. Lett. **111**, 243001 (2013); Phys. Rev. Lett. **113**, 073004 (2014)
- W. Nörtershäuser, C. Geppert, A. Krieger, K. Pachucki, M. Puchalski *et al.,* Phys. Rev. Lett. **115**, 033002 (2015)

New calculation: e.g. accuracy of $g_{\text{theo}}(^{12}\text{C}^{3+})$ improved $5\times$

- V. A. Yerokhin, K. Pachucki, M. Puchalski, Z. H., C. H. Keitel, Phys. Rev. A **95**, 062511 (2017)

Summary

- Accurate **test of QED** in strong fields with Si^{13+}
- Possibility to see nuclear effects
- Determining the **electron mass** with an order-of-magnitude improvement via the g-factor of C^{5+}
- New independent scheme for the improved determination of the **fine-structure constant** α in (near?) future from the g-factors of *light* H- and Li-like ions

Bedankt voor uw andacht!

Dziękuję za uwagę!

Grazie per l'attenzione!

Köszönöm a figyelmet!

Merci à tous pour votre attention!

Muchas gracias por su atención!

Mulţumesc pentru atenţie!

Obrigado pela atenção!

Спасибо за внимание!

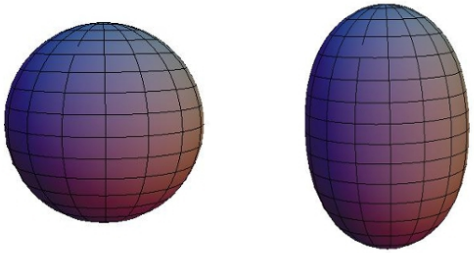
Thank you for your attention!

Vielen Dank für Ihre Aufmerksamkeit!

Additional slides

Nuclear effects – nuclear deformation

Some nuclei are deformed: angular dependence of the charge distribution



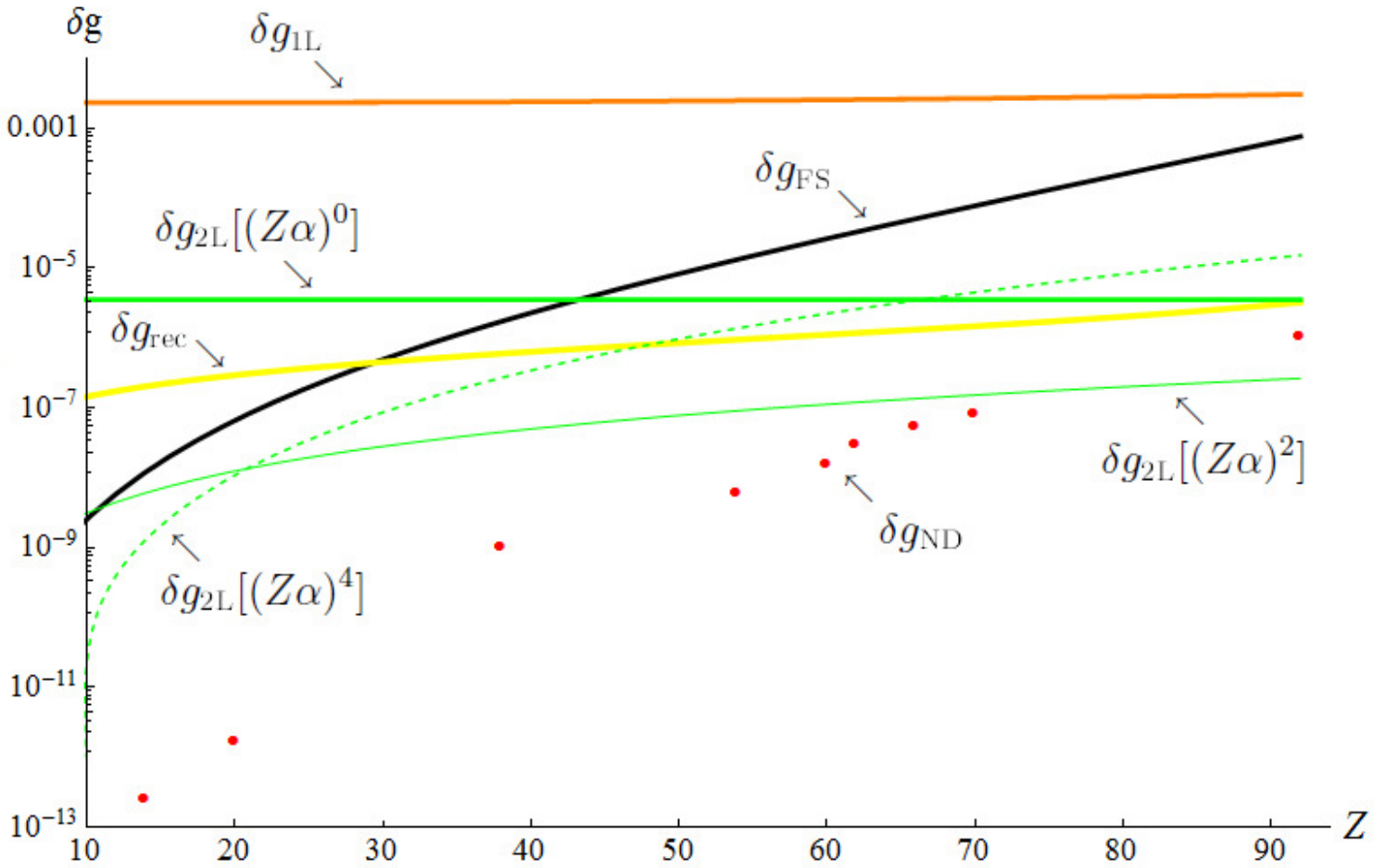
$$R(\theta,\phi) = R_0\left[1 + \beta_2 Y_{20}(\theta,\phi)\right]$$

$$\begin{aligned} \delta g_{\mathrm{ND}} &\propto -\beta_2^2 (Z\alpha)^4 \left(2mZ\alpha R\right)^{2\gamma}, \\ \gamma &= \sqrt{1-(Z\alpha)^2} \end{aligned}$$

Z	Isotope	β_2	δg_{ND}
6	^{12}C	0.44(10)	$-7.9(5.3)\cdot 10^{-16}$
14	^{28}Si	-0.349(20)	$-2.85(52)\cdot 10^{-13}$
	^{30}Si	-0.314(20)	$-2.48(49)\cdot 10^{-13}$
38	^{100}Sr	0.435(11)	$-1.08(28)\cdot 10^{-9}$
60	^{142}Nd	0.100(20)	$-2.0(1.1)\cdot 10^{-9}$
	^{150}Nd	0.278(20)	$-1.70(53)\cdot 10^{-8}$
62	^{144}Sm	0.090(20)	$-2.1(1.2)\cdot 10^{-9}$
	^{154}Sm	0.328(20)	$-3.24(98)\cdot 10^{-8}$
92	^{234}U	0.256(10)	$-1.12(27)\cdot 10^{-6}$
	^{238}U	0.280(10)	$-1.28(28)\cdot 10^{-6}$

- J. Zatorski, N. Oreshkina, C. H. Keitel, Z.H., Phys. Rev. Lett. **108**, 063005 (2012)

Comparison to other terms:



→ visible at the present relative exp. accuracy of $\approx 10^{-10}$

g factor of ions with non-zero nuclear spin

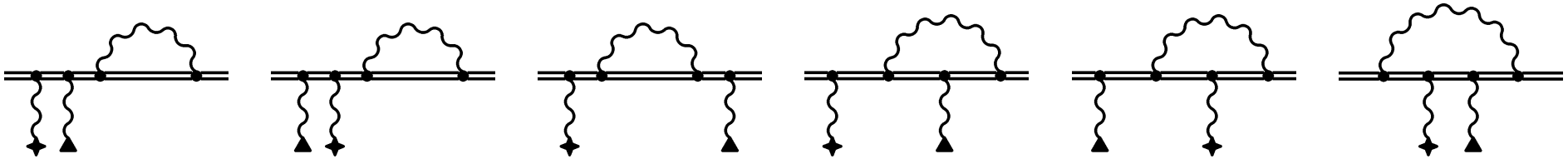
Total angular momentum of the electron: j, nuclear spin: I
Good angular momentum quantum number: F with $|I-j| \leq F \leq I+j$

$$g_F = g_j \frac{\mathbf{j}\cdot\mathbf{F}}{F(F+1)} - \frac{m}{m_p} g_I \frac{\mathbf{I}\cdot\mathbf{F}}{F(F+1)}$$

The interaction of the nuclear magnetic moment with the external magnetic field is modified by the presence of the bound electron: magnetic shielding

$$H = -\mu\mathbf{B}(1-\sigma) \Rightarrow g_I \rightarrow g_I(1-\sigma)$$

Feynman diagrams describing the shielding with SE corrections:

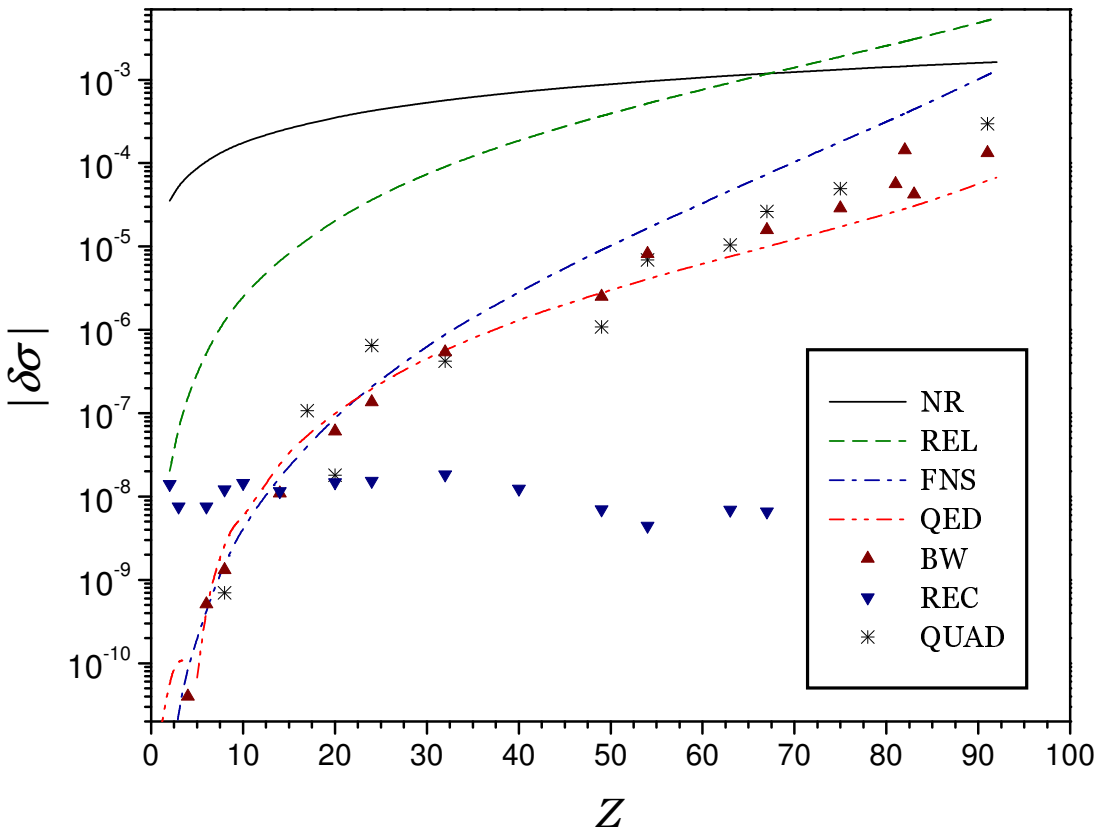


(a) (b) (c) (d) (e) (f)

The accurate knowledge of the shielding σ allows the extraction of the nuclear magnetic moment μ from (Penning trap) g factor measurements (relevant for e.g. NMR studies or nuclear structure):

$$\overline{g} \equiv g_{F=I+1/2} + g_{F=I-1/2} = -2\frac{m}{m_p}\frac{\mu}{\mu_N I}(1-\sigma)$$

Theoretical results for the contributions to σ:



- V. A. Yerokhin, K. Pachucki, Z.H., C. H. Keitel, Phys. Rev. Lett. **107**, 043004