The Bohr-Weisskopf effect and atomic parity violation

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Magdalena Kowalska
Jacek Dobaczewski

Motivation

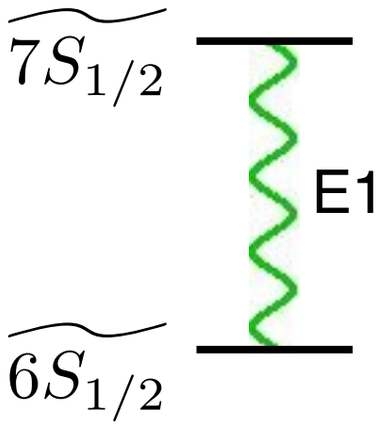
To maximise the discovery potential of APV measurements

- Push state-of-the-art atomic calculations to 0.1% precision
  - Development of precision atomic theory
  - Improved benchmarking of atomic theory
- Remove *nuclear structure uncertainties* to enable atomic theory tests below 0.1%

Atomic parity violation

Cs 6S-7S APV amplitude,
0.35% uncertainty

Carl Wieman group (1997)



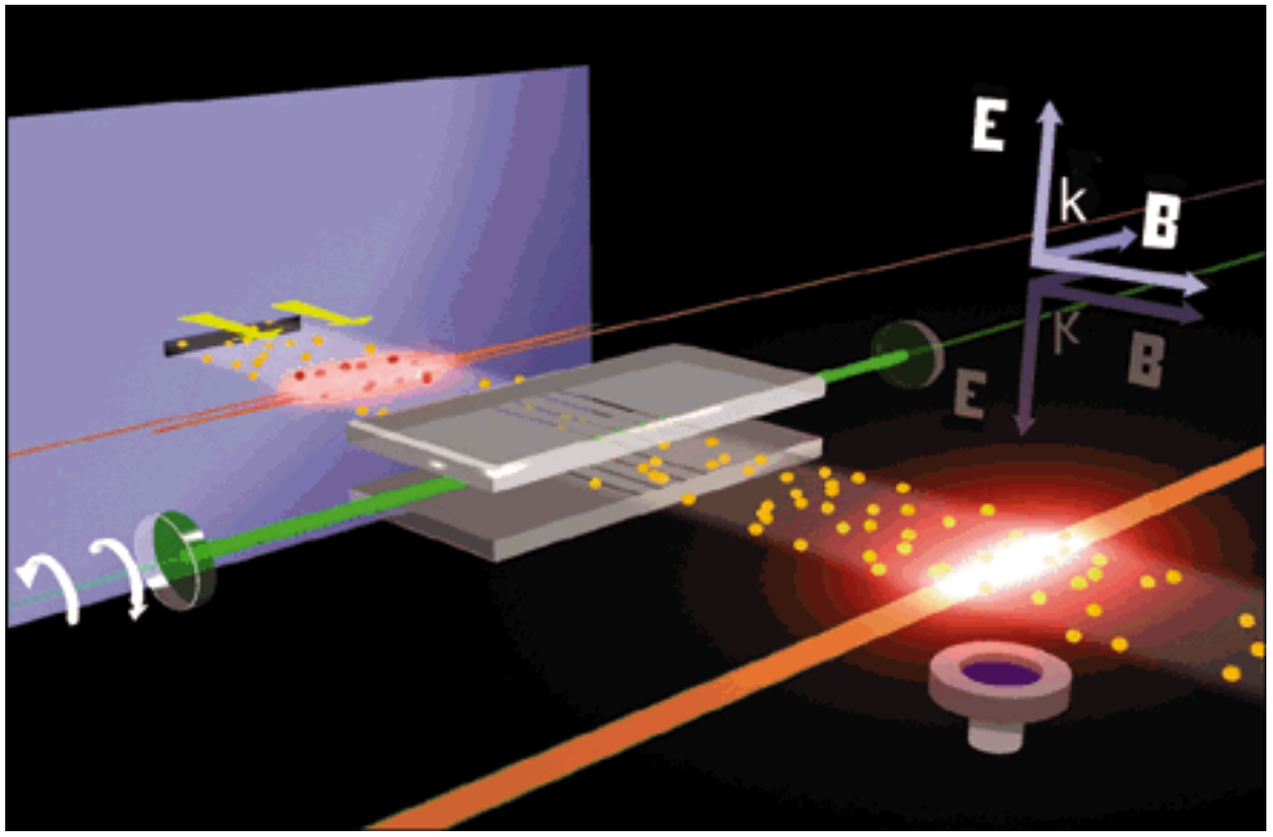
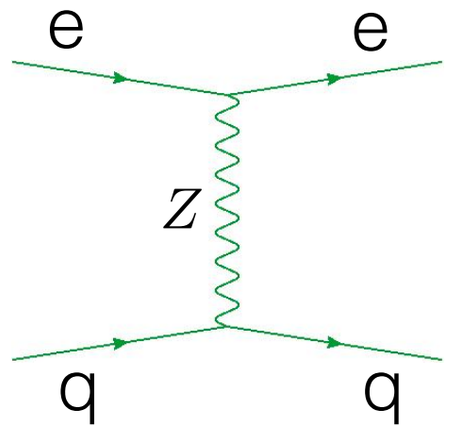


Image: T. Andrews, University of Colorado

$$\widetilde{S_{1/2}} \rightarrow S_{1/2} + \sum \zeta \, nP_{1/2}$$

Parity-violating weak interaction, $h_{\mathrm{PV}} = -\frac{G_F}{2\sqrt{2}} Q_W \rho(r) \gamma_5$

$E_{\mathrm{PV}} \propto Z^3$



Bouchiat, Bouchiat, J. Phys. (Paris), 899 (1974)

Atomic parity violation

Cs 6S-7S APV amplitude,
0.5% uncertainty

Most precise calculations:

- Dzuba, Flambaum, Ginges, PRD (2002); Flambaum, Ginges, PRA (2005)
- Porsev, Beloy, Derevianko, PRL (2009); Dzuba, Berengut, Flambaum, Roberts, PRL (2012)

$$
\begin{aligned}
E_{\mathrm{PV}} &= \langle \widetilde{7S_{1/2}} | D_z | \widetilde{6S_{1/2}} \rangle \\
&= \sum_n \frac{\langle 7S_{1/2} | D_z | nP_{1/2} \rangle \langle nP_{1/2} | H_{\mathrm{PV}} | 6S_{1/2} \rangle}{E_{6S_{1/2}} - E_{nP_{1/2}}} \\
&\quad + \ldots \\
&= \xi \, Q_W
\end{aligned}
$$

Dipole operator	Weak operator	Energies
$\mathbf{D} = \sum_i e\mathbf{r}_i$	$H_{\mathrm{PV}} = \sum_i (h_{\mathrm{PV}})_i$	E

Recent calculation: Sahoo and Das [Sahoo, Das, Spiesberger, PRD(L) (2021)]*

Working towards 0.1-0.2% precision:

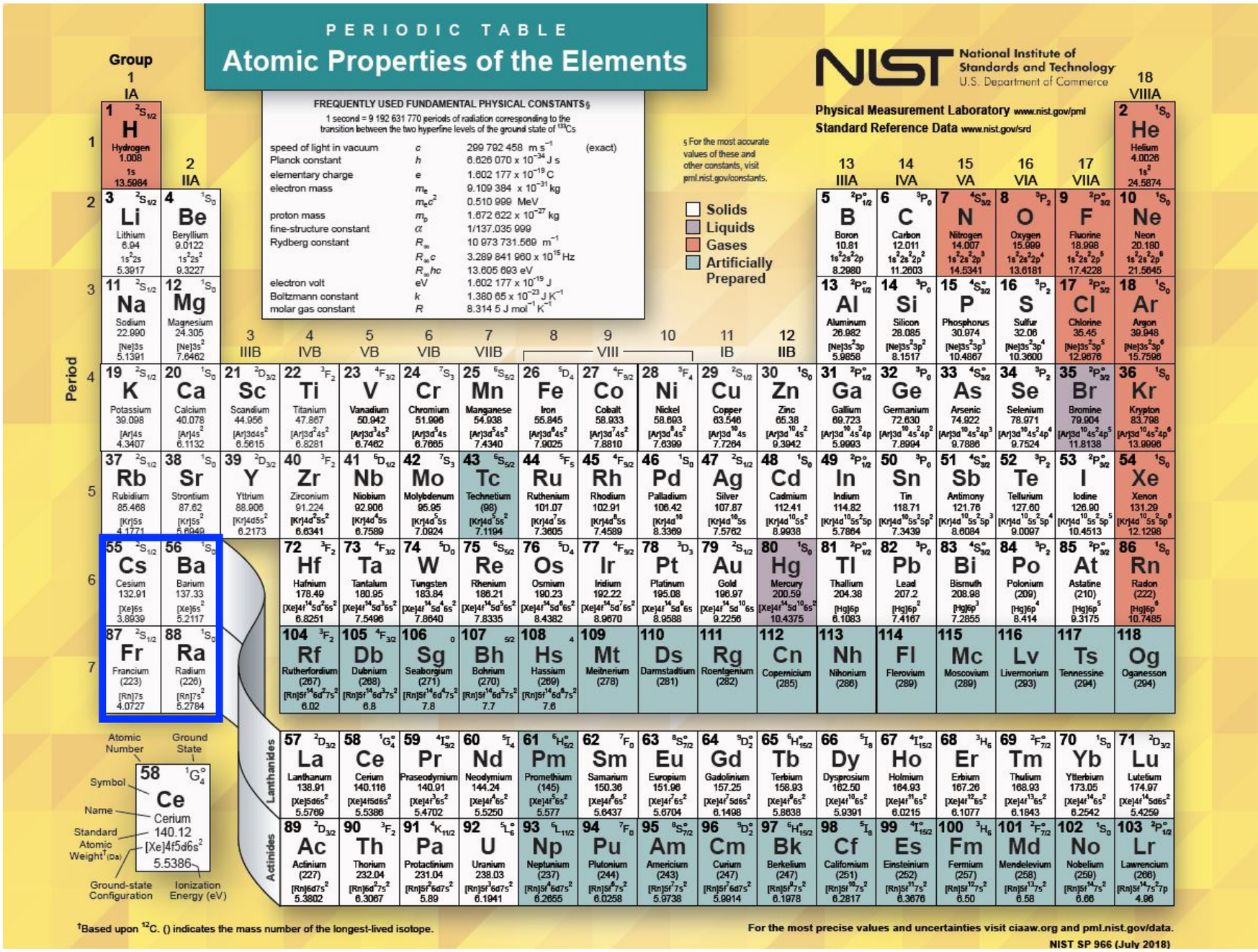
- Precision Atomic Theory group @ UQ
- Derevianko's group [Tran Tan, Xiao, Derevianko, PRA (2022)]

*Comment: Roberts and Ginges, PRD (2022)

Atomic parity violation

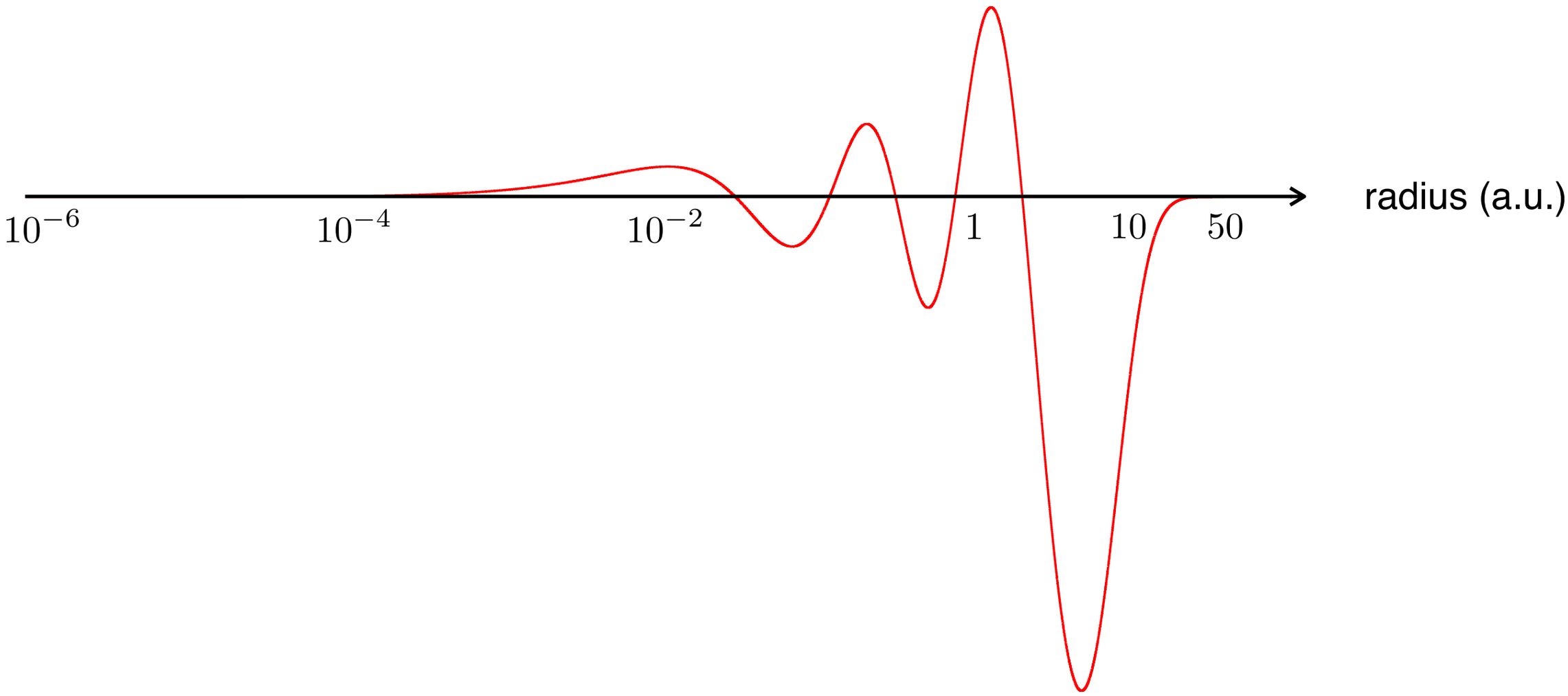
Experiments in preparation/progress include:

- Cs (Purdue)
- Fr (TRIUMF; Tokyo)
- Ba^+ (Seattle)
- Ra^+ (Groningen)



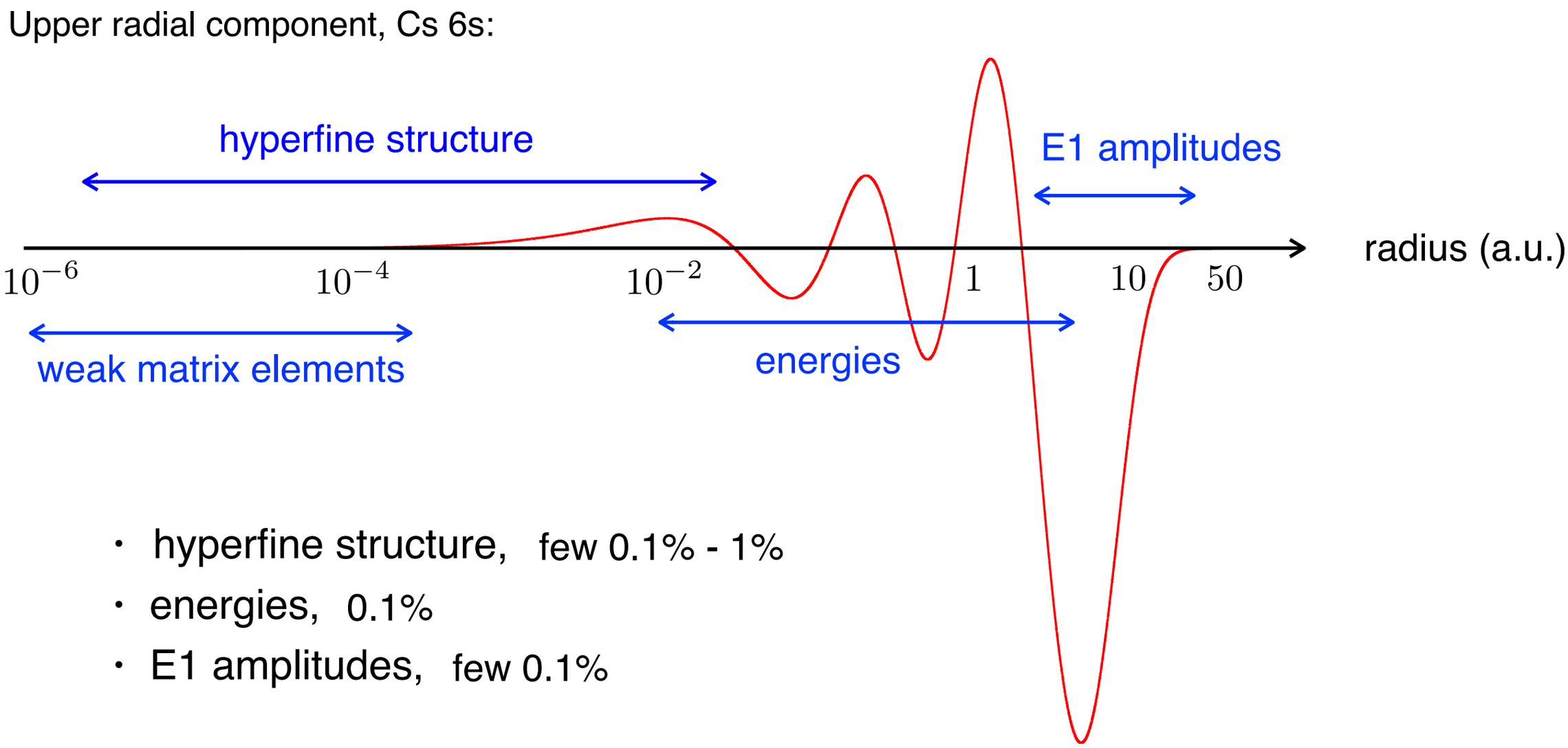
Benchmarking atomic theory

Upper radial component, Cs 6s:



$$E_{\rm PV} = \sum_n \frac{\langle 7S_{1/2}|D|nP_{1/2}\rangle\langle nP_{1/2}|H_{\rm PV}|6S_{1/2}\rangle}{E_{6S_{1/2}} - E_{nP_{1/2}}} + \sum_n \frac{\langle 7S_{1/2}|H_{\rm PV}|nP_{1/2}\rangle\langle nP_{1/2}|D|6S_{1/2}\rangle}{E_{7S_{1/2}} - E_{nP_{1/2}}} = \xi Q_W$$

Benchmarking atomic theory



- hyperfine structure, few 0.1% - 1%
- energies, 0.1%
- E1 amplitudes, few 0.1%

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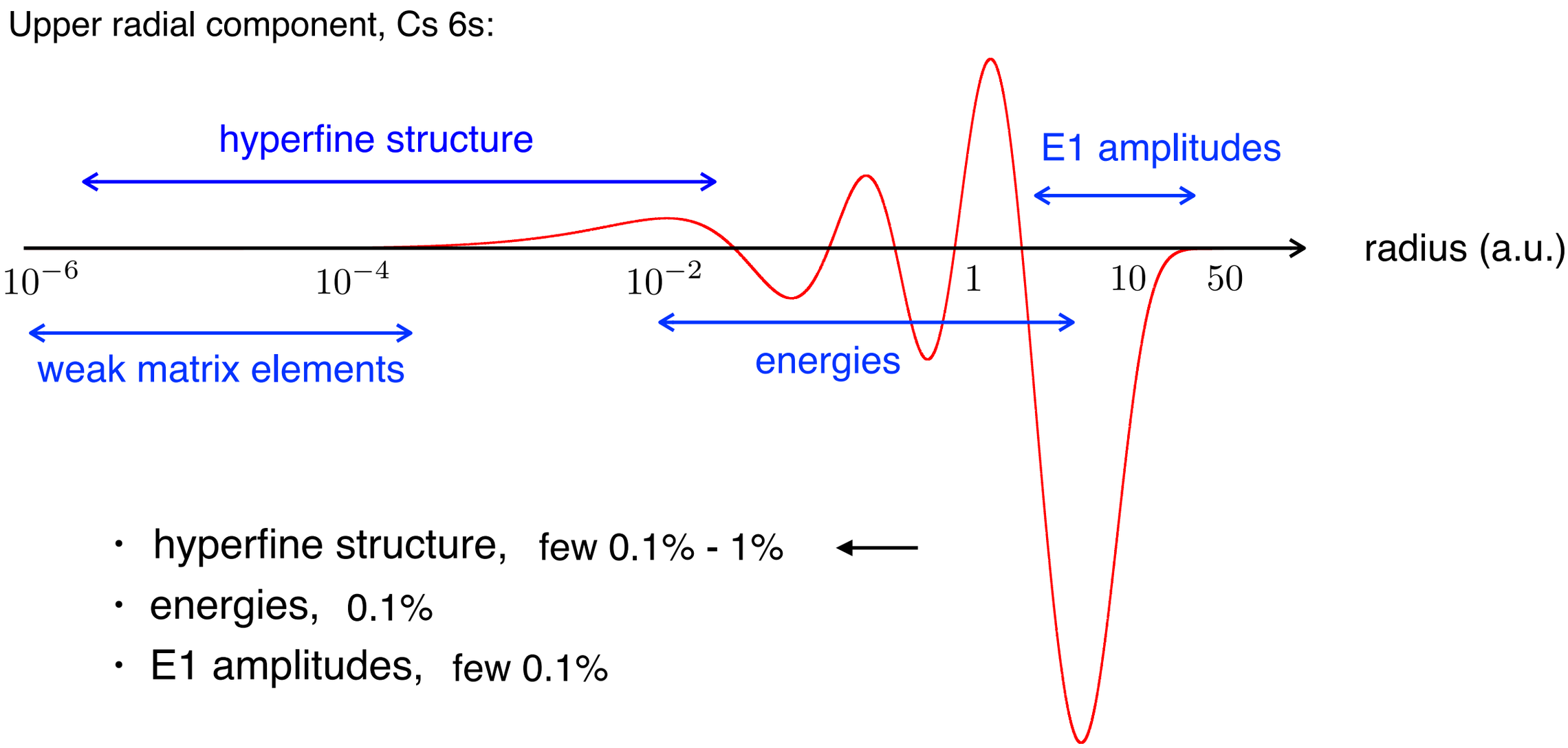
Benchmarking atomic theory



- hyperfine structure, few 0.1% - 1% ⟵
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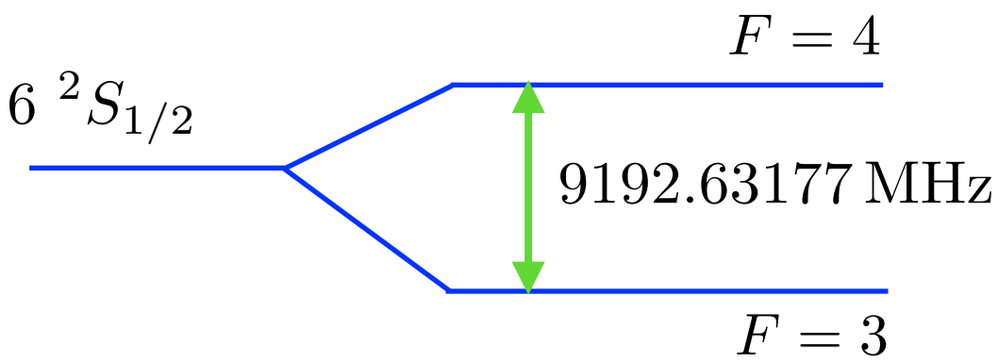
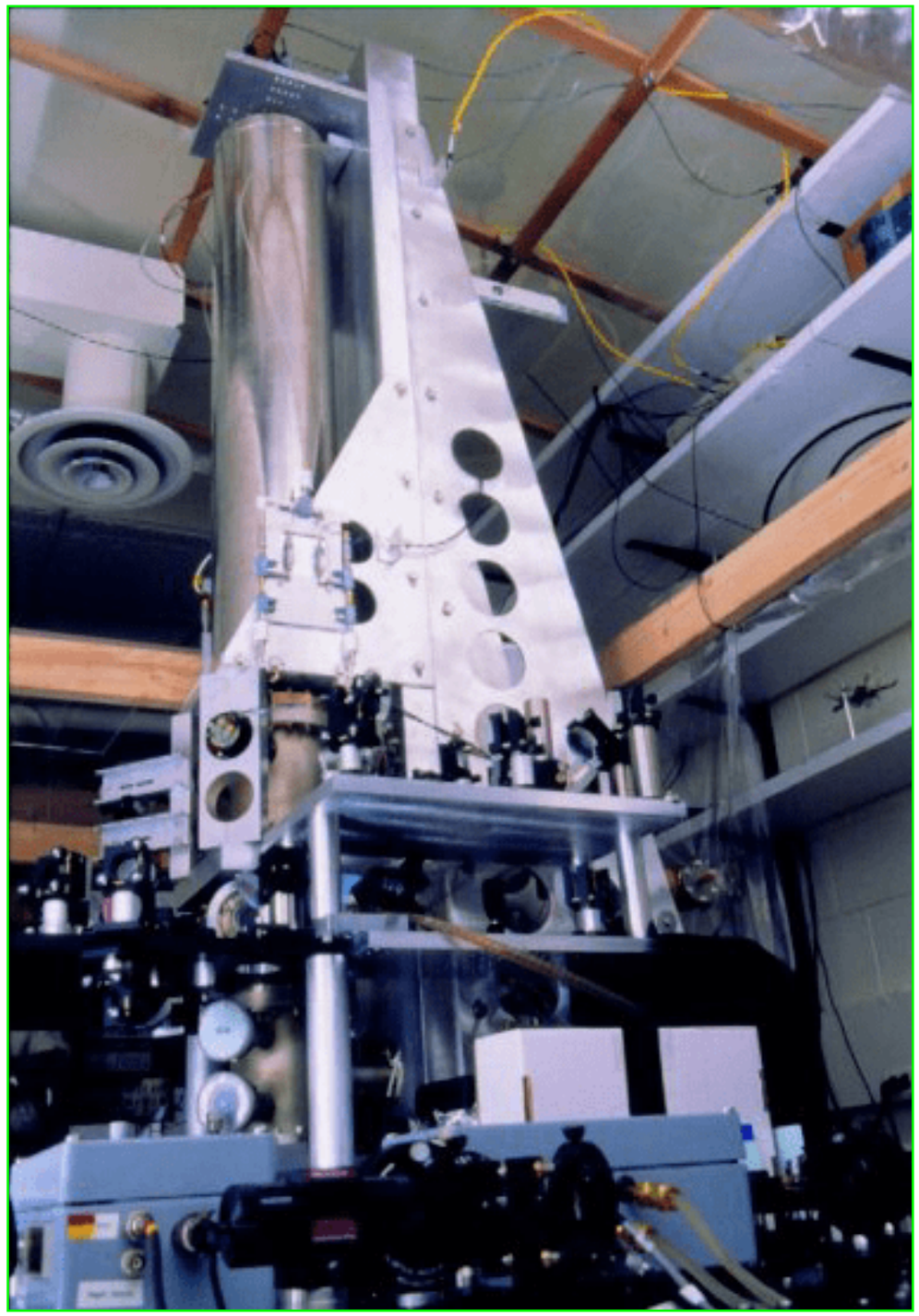
Hyperfine structure

NIST-F2 Atomic clock

Primary standard for the SI unit for time, the *second*

Hyperfine splitting in cesium





Hyperfine structure

Modelling the hyperfine structure

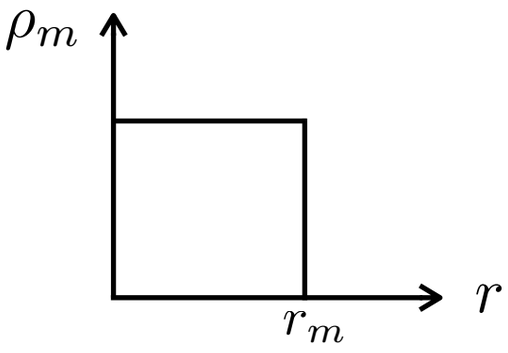
nuclear magnetic moment
$\mu = \mu \mathbf{I}/I$

Interaction $$h_{\rm hfs} = \frac{1}{c}\frac{\boldsymbol{\mu}\cdot(\mathbf{r}\times\boldsymbol{\alpha})}{r^3}F(r)$$

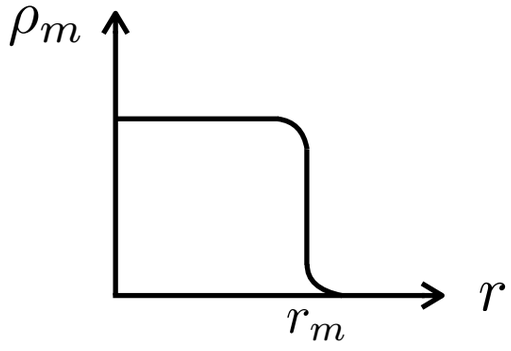
describes the nuclear magnetization distribution

For a point-nucleus $F(r) = 1$

Ball, $F(r) = (r/r_m)^3$



Fermi distribution



Standard ways to model *F(r)*, until recently:

Hyperfine splitting quantified by hyperfine constant *A*

$$A = A_0(1+\epsilon) + \delta A^{\rm QED}$$

↑

Many-body result,
finite nuclear charge effect included

Hyperfine structure

Modelling the hyperfine structure

nuclear magnetic moment
$\mu = \mu \mathbf{I}/I$

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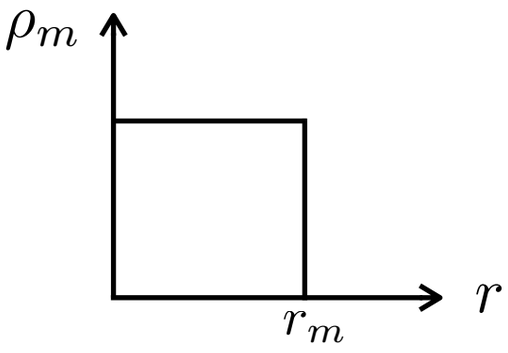

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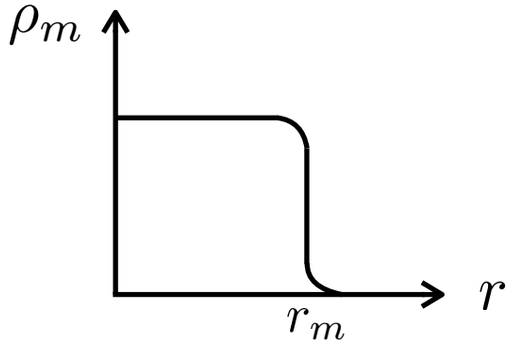

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Bohr-Weisskopf (BW) effect —
finite nuclear magnetization contribution

Hyperfine structure

Modelling the hyperfine structure

nuclear magnetic moment
$\mu = \mu \mathbf{I}/I$

Interaction $$h_{\rm hfs} = \frac{1}{c}\frac{\boldsymbol{\mu}\cdot(\mathbf{r}\times\boldsymbol{\alpha})}{r^3}F(r)$$

describes the nuclear magnetization distribution

For a point-nucleus $F(r) = 1$

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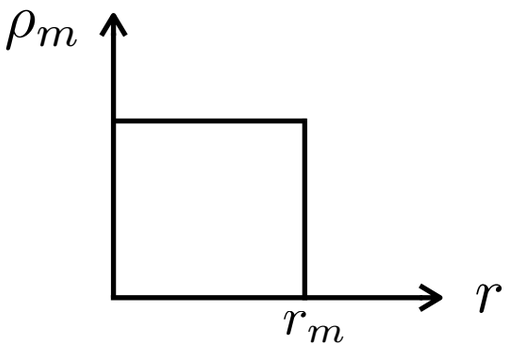

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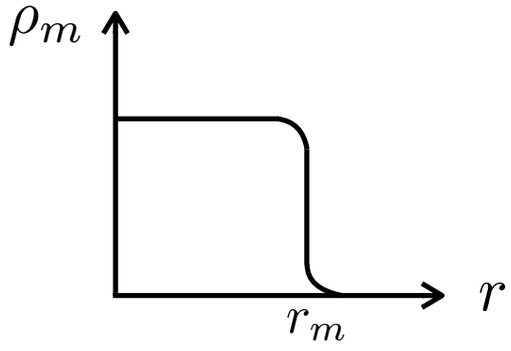

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Quantum electrodynamics radiative correction

Hyperfine structure

Modelling the hyperfine structure

nuclear magnetic moment
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Interaction $$h_{\rm hfs} = \frac{1}{c}\frac{\boldsymbol{\mu}\cdot(\mathbf{r}\times\boldsymbol{\alpha})}{r^3}F(r)$$

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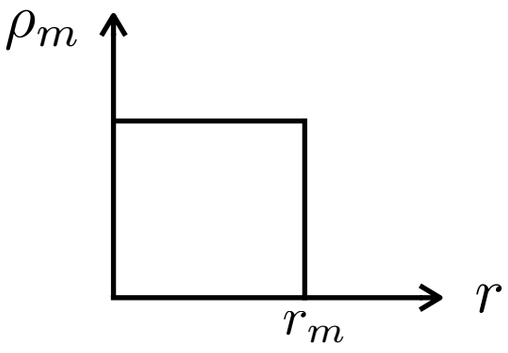

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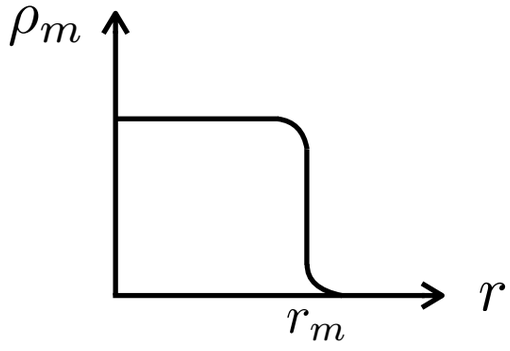


Standard ways to model *F(r)*, until recently:

Hyperfine splitting quantified by hyperfine constant *A*

$$A = A_0(1+\epsilon) + \delta A^{\rm QED}$$

contains factor μ

Hyperfine structure

Hyperfine comparisons

$$A^{\rm expt} \longleftrightarrow A_0(1+\epsilon) + \delta A^{\rm QED}$$

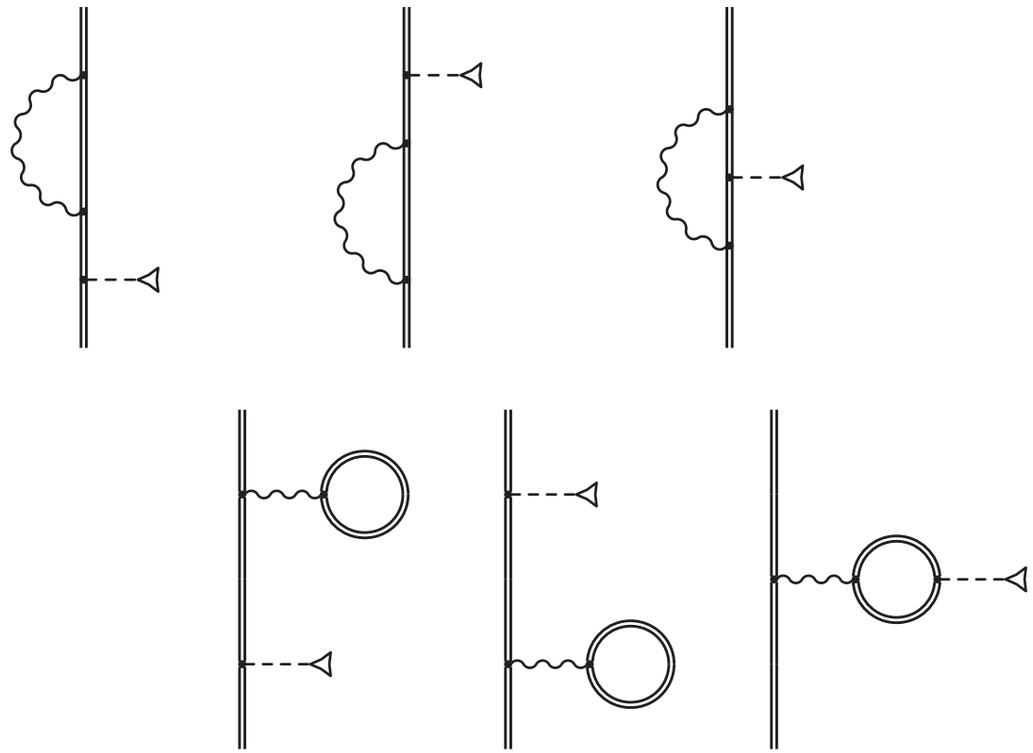
Provides test of atomic many-body theory in the nuclear vicinity *only if*

- Nuclear magnetic moments μ
- Bohr-Weisskopf effect ϵ
- QED radiative corrections $\delta A^{\rm QED}$

are known well (contributing < 0.1% uncertainty to hyperfine constants)

Hyperfine structure

<u>QED corrections</u>



Self-energy and vacuum polarisation corrections evaluated for:

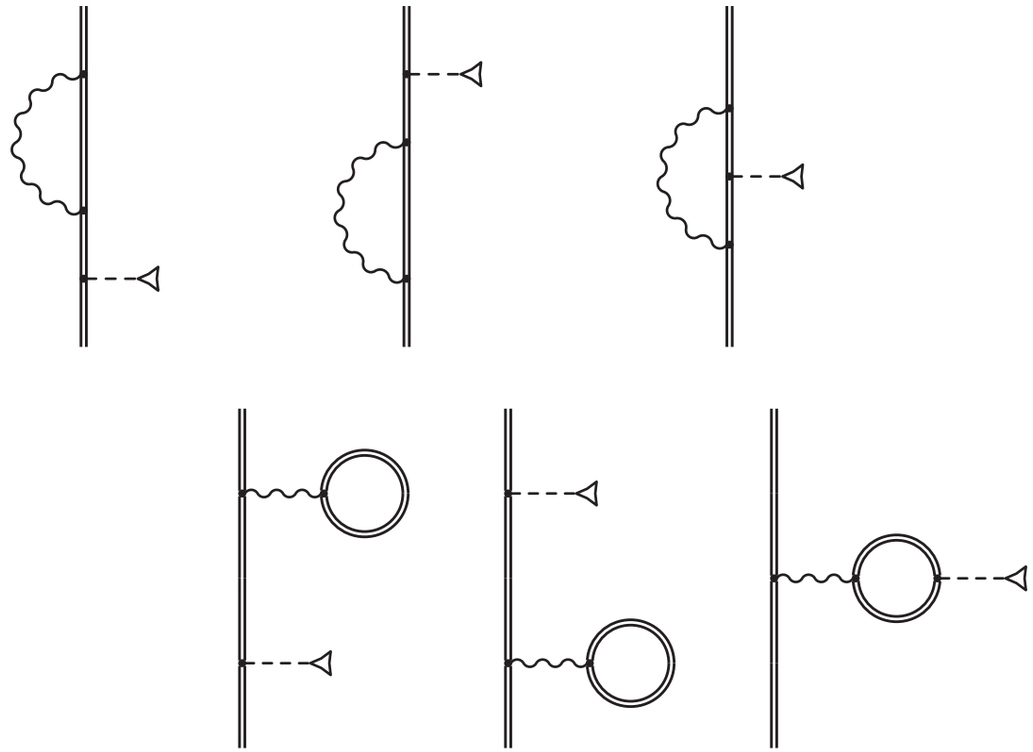
- lowest states of alkali-metal atoms;
- ground-states of Rb, Cs, Fr, Ba^+, Ra^+

QED corrections (%) to ground state hyperfine constants

Cs	Ba^+	Fr	Ra^+	Reference
-0.38(6)	-0.37(4)	-0.60(1)	-0.55(8)	Ginges, Volotka, Fritzsche, PRA (2017)
-0.42		-0.6		Sapirstein and Cheng, PRA (2003)

Hyperfine structure

<u>QED corrections</u> ✔



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Hyperfine structure

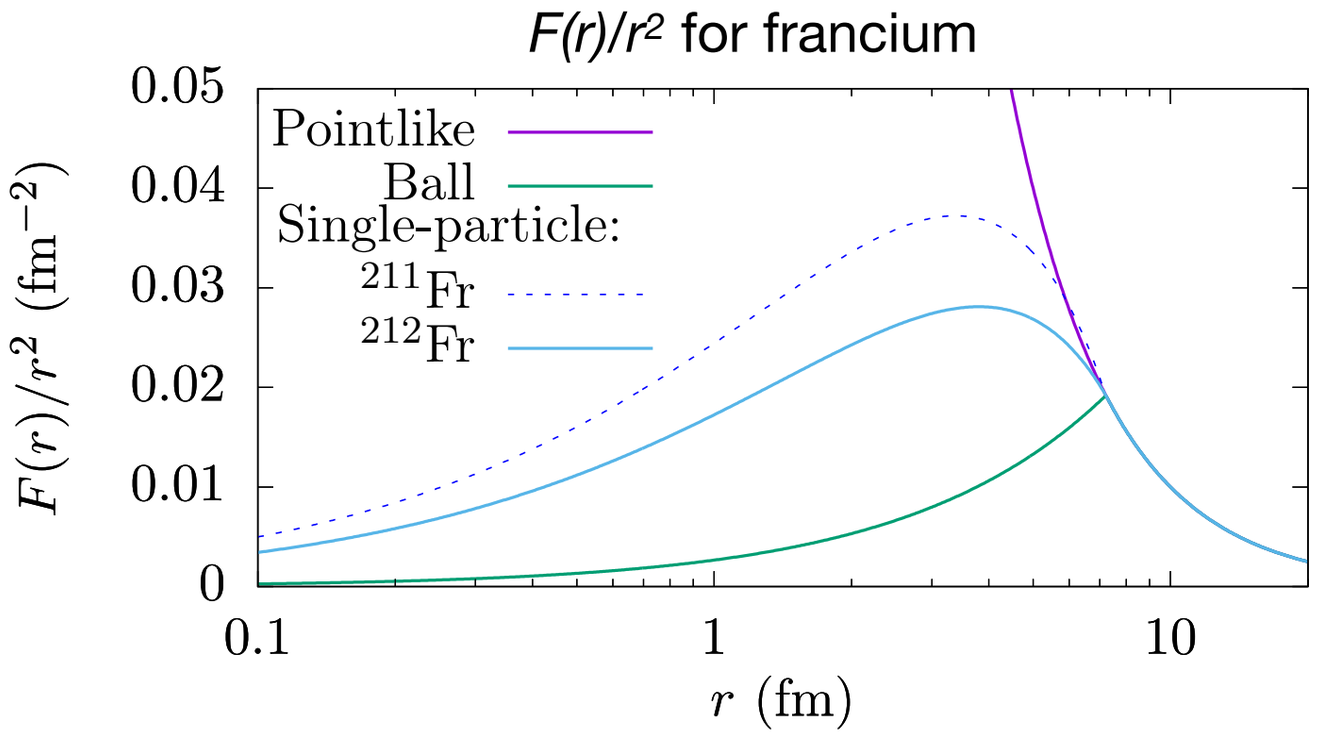
Bohr-Weisskopf (BW) effect

$$\epsilon = \frac{\int_0^{r_m} dr f(r) g(r) [F(r) - 1]/r^2}{\int_0^{\infty} dr f(r) g(r)/r^2}$$

Single-particle model:

g_S found from measured nuclear magnetic moment using Lande factor

$$F(r) = \left(\frac{r}{r_m}\right)^3 \left[1 - 3\ln\left(\frac{r}{r_m}\right) \frac{\mu_N}{\mu} \left(-\frac{2I-1}{8(I+1)} g_S + \frac{2I-1}{2} g_L\right)\right] \quad \text{for } I=L+1/2$$



nuclear model	^{133}Cs	^{135}Ba$^+$	^{211}Fr	^{225}Ra$^+$
ball	-0.71	-0.74	-2.7	-2.8
single-particle	-0.21	-1.0	-1.3	-2.8
single-particle (WS, spin-orbit)	-0.19(14)	-1.3(4)	-1.4(5)	-4.3(13)

BW corrections (%) to s-state hyperfine constants

Expression for F(r): Volotka *et al.,* PRA (2008)
Ginges, Volotka, Fritzsche , PRA (2017)

Hyperfine structure

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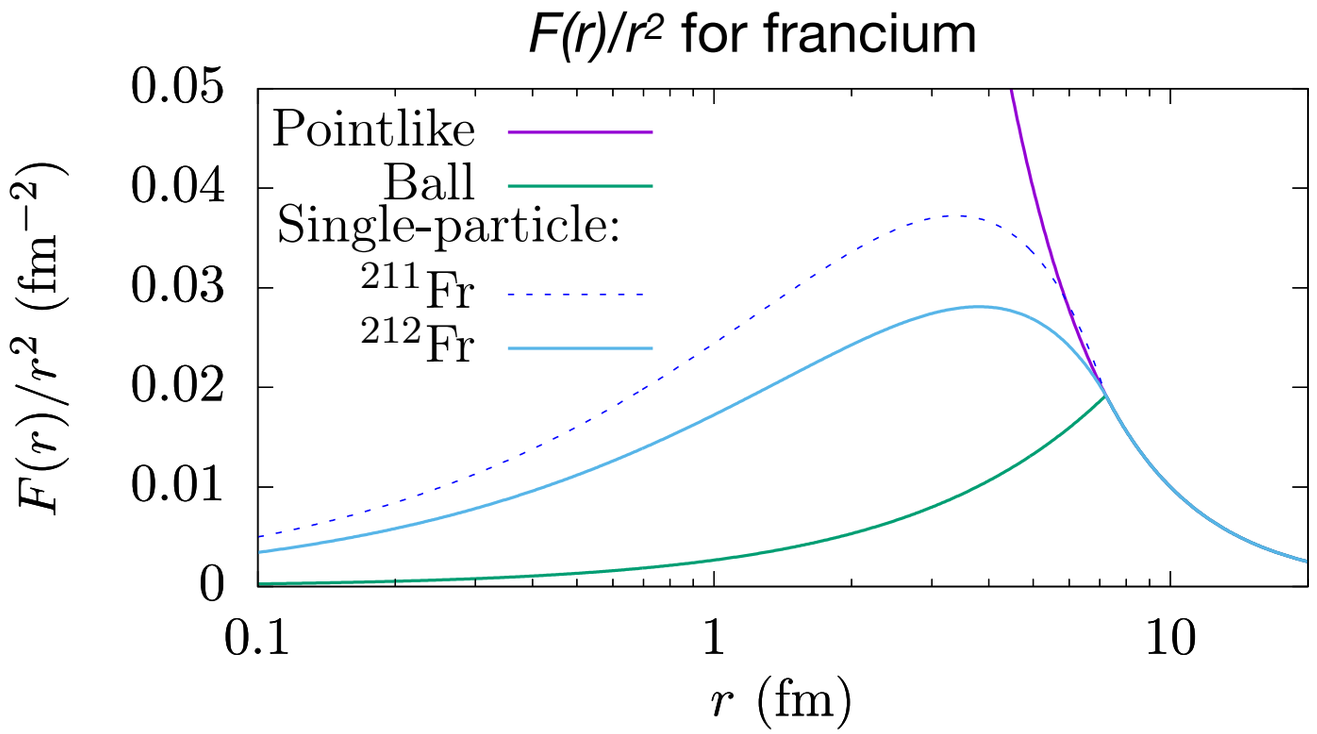

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Difference	**0.5%**		**1.3%**	

BW corrections (%) to hyperfine constants

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Hyperfine structure

Bohr-Weisskopf (BW) effect ✗

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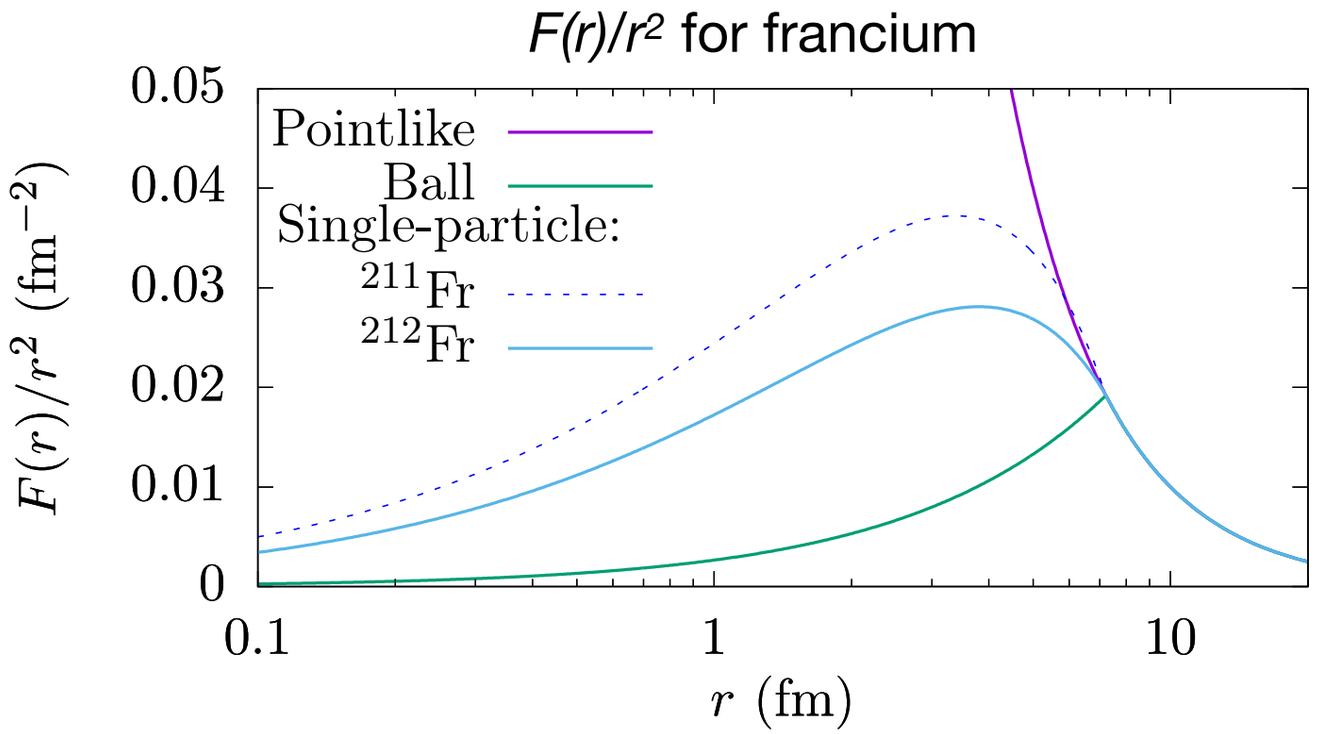

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BW corrections (%) to hyperfine constants

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Hyperfine structure

Calculations of hyperfine intervals and comparison with experiment. Units: MHz

	^{133}Cs	^{135}Ba^{+}	^{211}Fr	^{225}Ra^{+}
Many-body	9229.5	7286.8	45374	-29113
BW	-17.0(131)	-91.8(275)	-641(244)	1267(380)
QED	-35.1(58)	-27.1(30)	-273(56)	159(23)
Total theory	9177.4	7167.9	44460	-27687
Experiment	9192.6	7183.3	43570	-27731
Difference	-15.2	-15.4	890	44
Difference (%)	-0.17(16)	-0.21(38)	2.0(6)(20)	-0.2(14)

Ginges, Volotka, Fritzsche, PRA (2017)

Hyperfine structure

Nuclear magnetic moments

How well do we know μ? ^{133}Cs, ^{135}Ba, Fr isotopes, ^{225}Ra

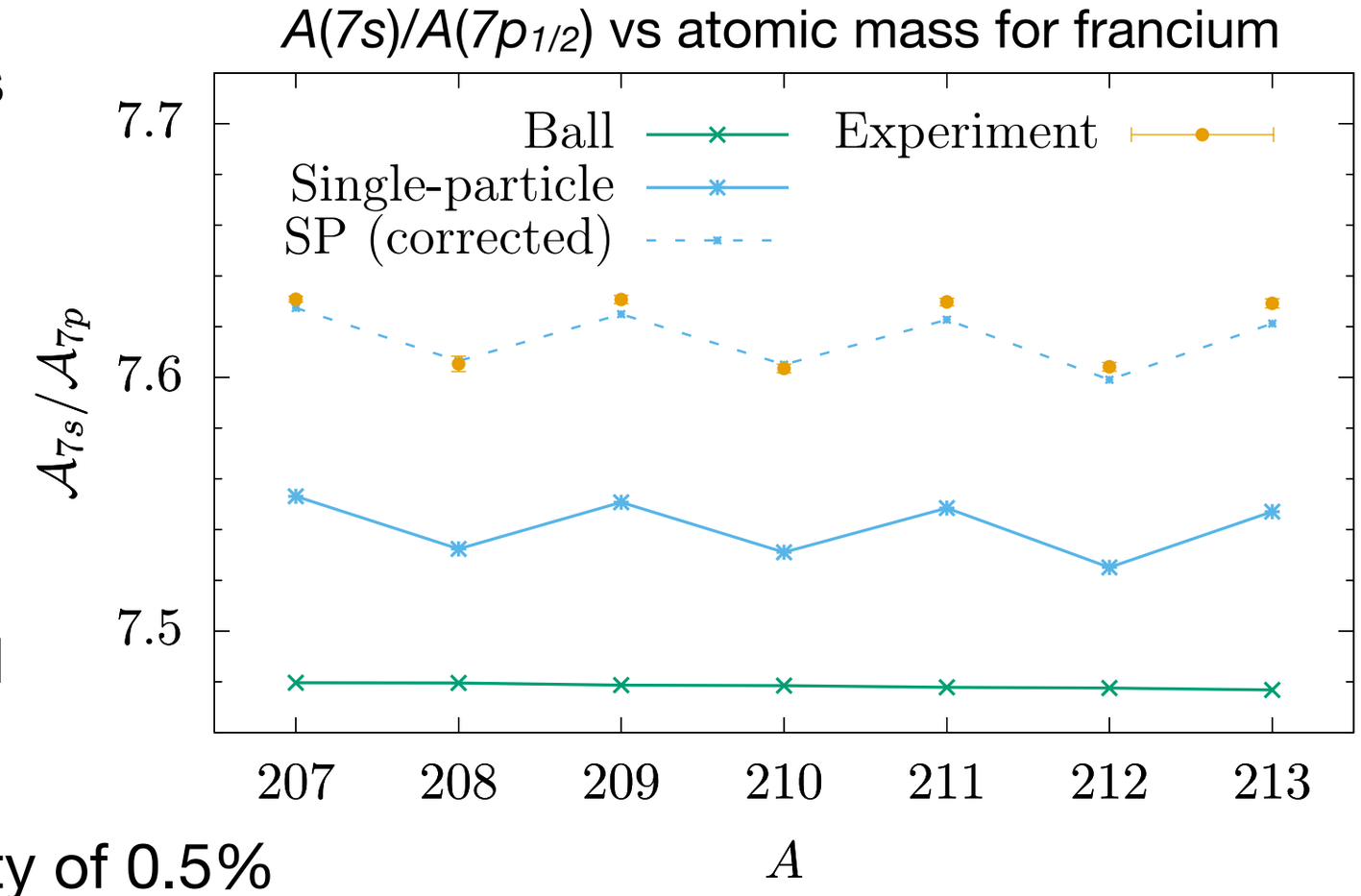
uncertainties: negligible 1-2% 0.2%

Our atomic theory uncertainty is better $\Rightarrow$ can find μ(Fr)!

$$A^{\text{expt}} \longleftrightarrow A^{\text{th}}(\mu_{\text{th}})(\mu/\mu_{\text{th}})$$

Test/control BW effect using:

- ratios of *A* for different states
- Empirical BW value extracted from H-like ^{209}Bi



Determined μ with an uncertainty of 0.5%

Roberts and Ginges, PRL (2020)

Hyperfine structure

Nuclear magnetic moments ✔

How well do we know μ? ^{133}Cs, ^{135}Ba, Fr isotopes, ^{225}Ra

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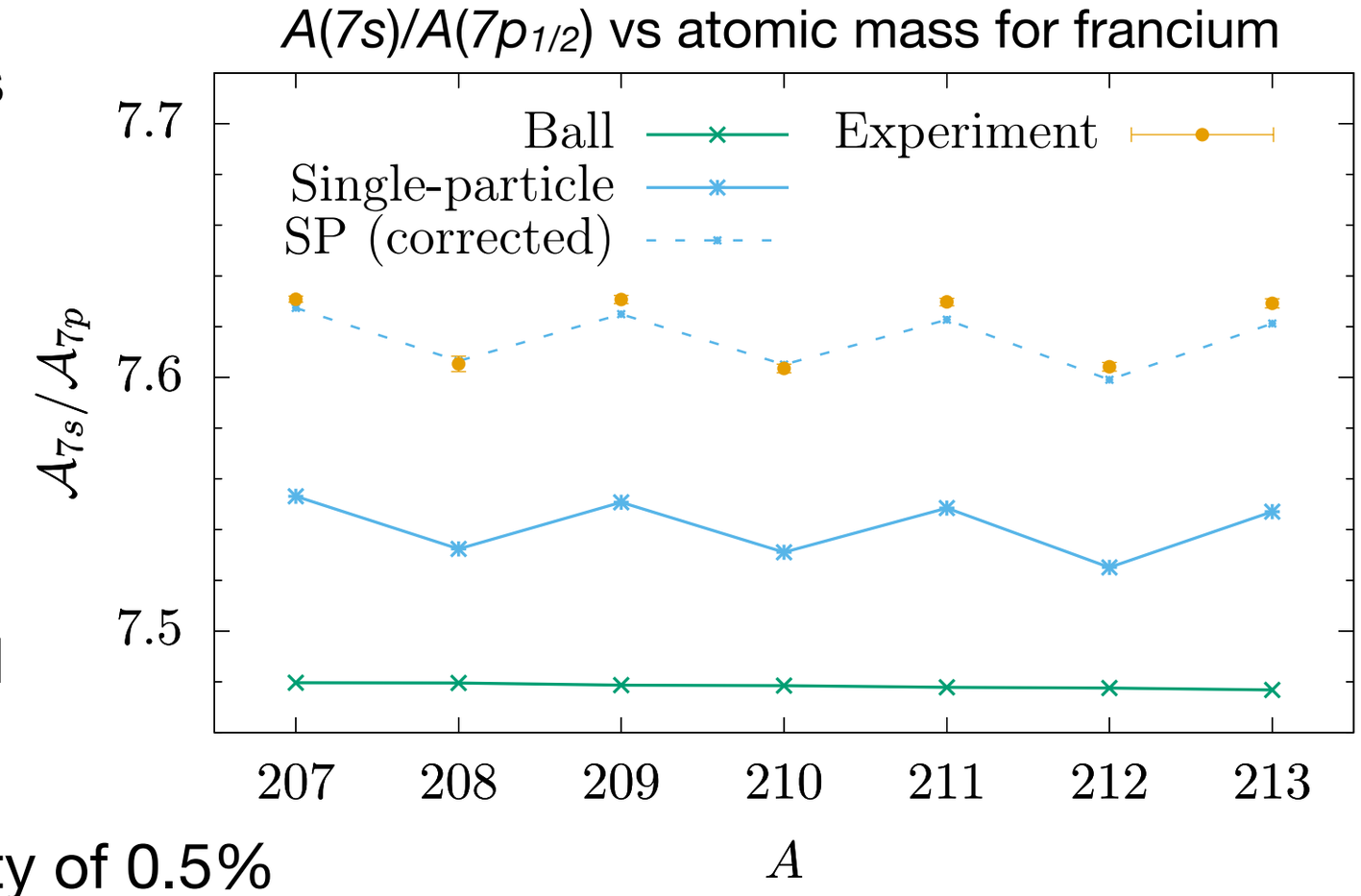

Roberts and Ginges, PRL (2020)

Hyperfine structure

Nuclear magnetic moments ✔ ✗

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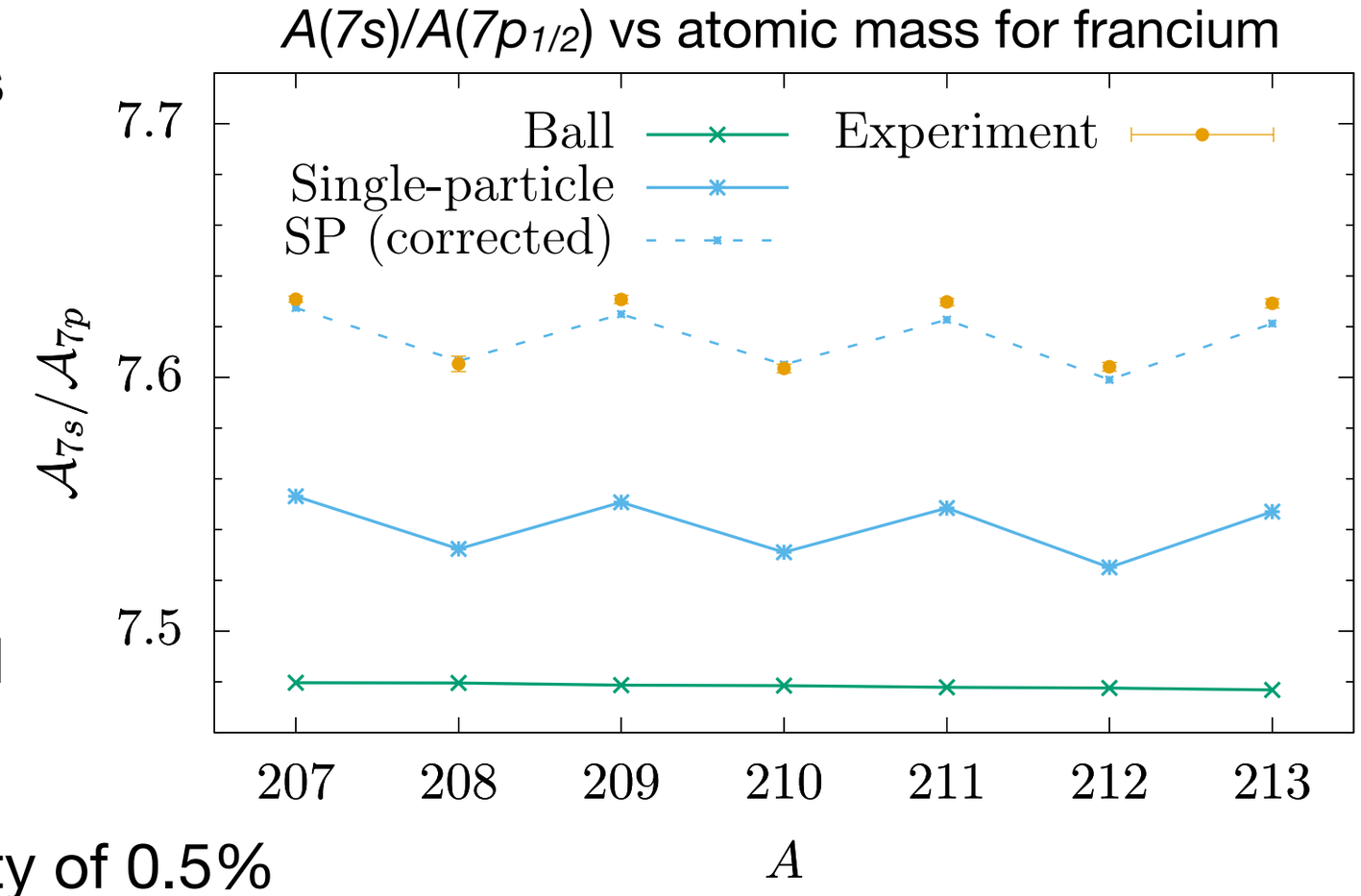

Determined μ with an uncertainty of 0.5%

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Bohr-Weisskopf effect

Properties

Relative BW correction $$\epsilon = \frac{\int_0^{r_m} dr f(r) g(r) [F(r) - 1]/r^2}{\int_0^{\infty} dr f(r) g(r)/r^2}$$

In the nuclear region, the electrons see the unscreened Coulomb field of the nucleus. Since the binding energies $\varepsilon \ll V(r)$, wave functions with the same angular dependence are proportional.

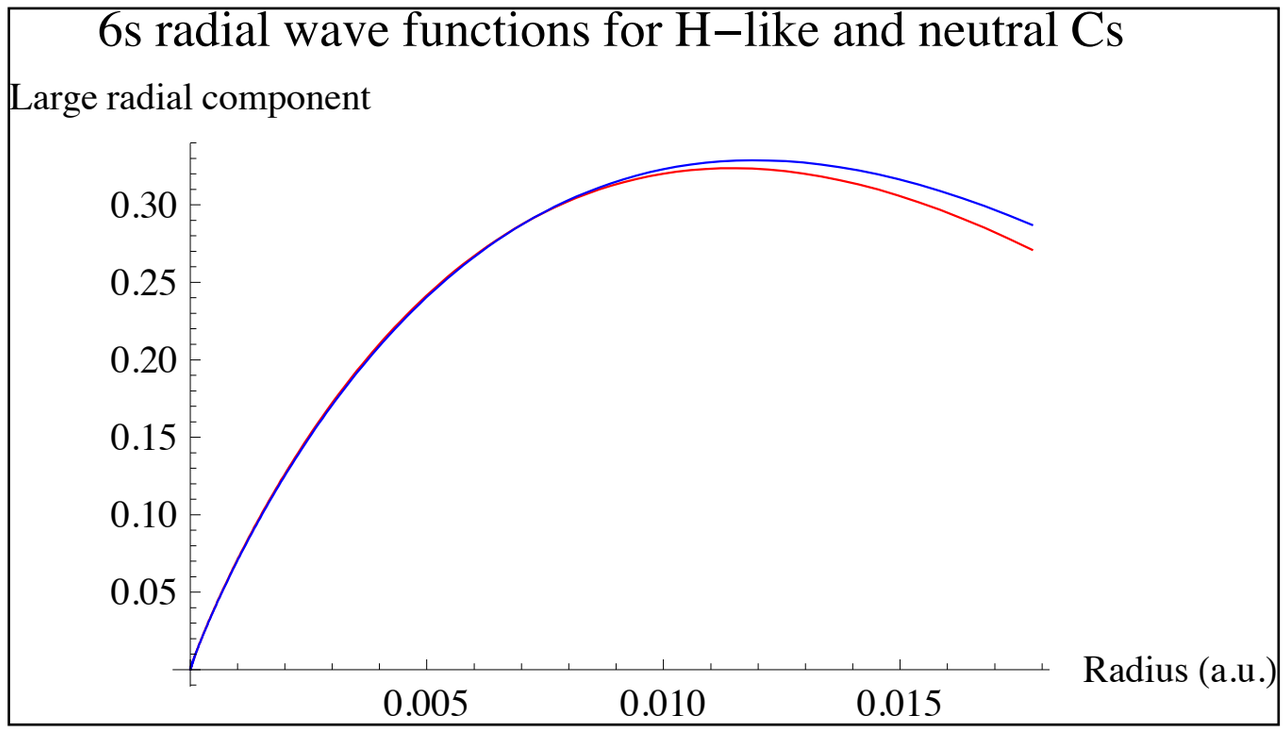
$$\begin{bmatrix} V(r) - \varepsilon & c(\kappa/r - \partial_r) \\ c(\kappa/r + \partial_r) & V(r) - \varepsilon - 2c^2 \end{bmatrix} \begin{bmatrix} f_{n\kappa} \\ g_{n\kappa} \end{bmatrix} = 0$$

BW effect is independent of principal quantum number!

$$\Rightarrow \quad \epsilon_{n\kappa} = \epsilon_{n'\kappa}$$

Also, in the nuclear region, for heavy systems:

$$f_{s_{1/2}} \propto g_{p_{1/2}} \quad , \quad f_{p_{1/2}} \propto g_{s_{1/2}}$$



BW effects in atoms related to BW matrix element for *1s* state of H-like ion

Skripnikov, J. Chem. Phys. (2020)
Roberts and Ginges, PRA (2022)

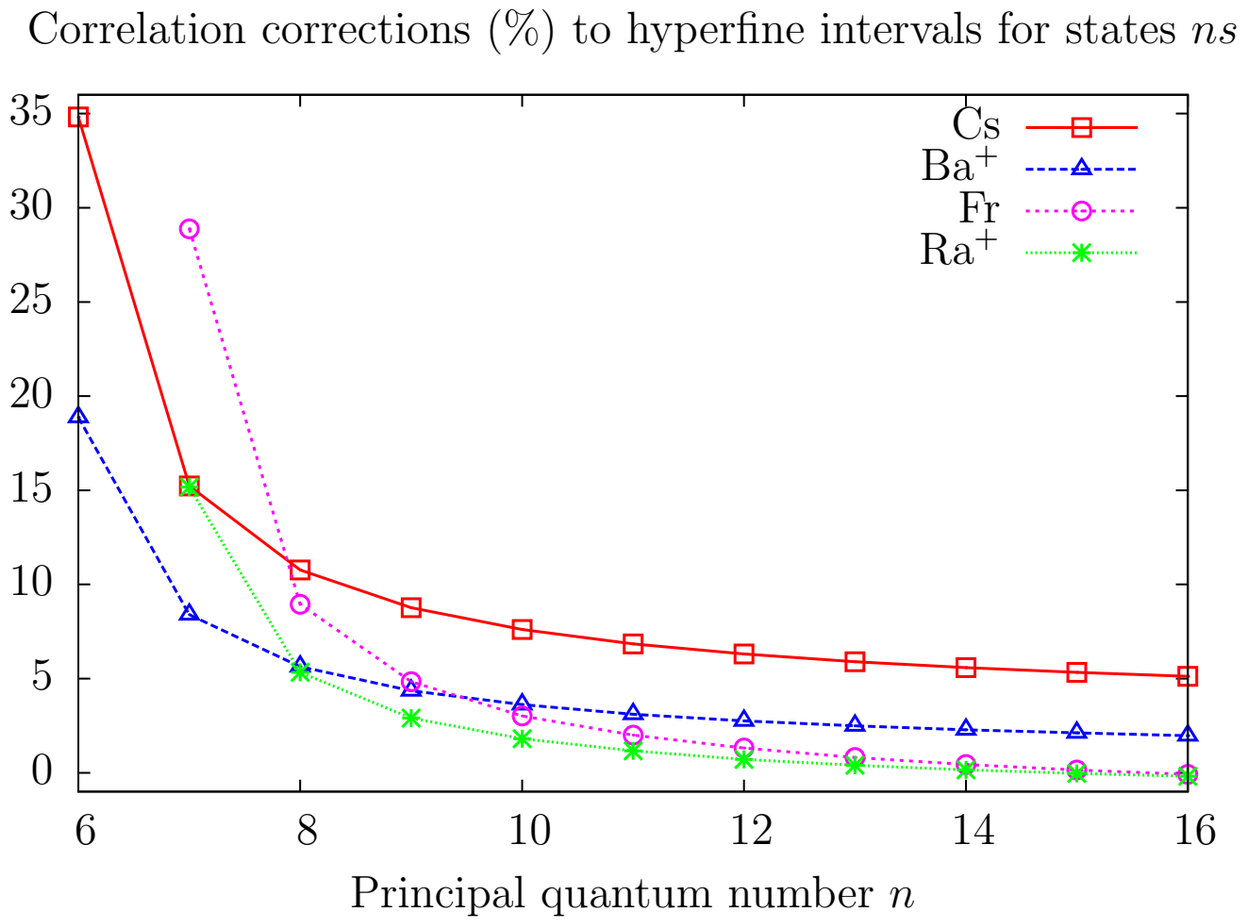
Bohr-Weisskopf effect

<u>To remove or extract?</u>

<u>Ratio method</u>

By taking a ratio of two states with different principal quantum number, the dependence on the BW effect may be removed!

$$A^{\rm th}_{n\kappa} = A_{0,n\kappa}\left(A^{\rm exp}_{n'\kappa}/A_{0,n'\kappa}\right)$$



	$A_{\rm hfs}$ (MHz)			
	Experiment		Theory	
State	This work	Prior expt.	Ref. [37]	Ref. [16]
12s	26.318 (15)	26.31 (10) [24]	26.28	26.30 (2)
13s	18.431 (10)	18.40 (11) [25]		18.42 (1)

This may be used to make high-precision predictions of the hyperfine constants!

Ratio method: Ginges and Volotka, PRA (2018)
Ref. [16] Grunefeld, Roberts, Ginges, PRA (2019)
Experiment: Quirk et al., PRA (2022)

Bohr-Weisskopf effect

Differential hyperfine anomaly

Ratio of hyperfine constants of different isotopes of the same element,

$$\mathcal{A}^{(1)}/\mathcal{A}^{(2)} = g_I^{(1)}/g_I^{(2)}(1 +^1 \Delta^2) \ ,$$

and typically for nuclei of different spin,

$$^1\Delta^2 \approx \epsilon^{(1)} - \epsilon^{(2)} \ .$$

Gives the *difference* in the BW effect for different isotopes.

		Isotope 1				Isotope 2				Differential anomaly $^1\Delta^2$ (%)		
		A	I^π	ϵ_{Ball} (%)	ϵ_{SP} (%)	A	I^π	ϵ_{Ball} (%)	ϵ_{SP} (%)	Ball	SP	Expt. [59]
$_{37}$Rb	$5s_{1/2}$	85	$5/2^-$	−0.306	0.044	87	$3/2^-$	−0.306	−0.278	−0.001	0.323	0.35142(30)
						86	2^-	−0.306	−0.139	0.000	0.183	0.17(9)
$_{47}$Ag	$5s_{1/2}$	107	$1/2^-$	−0.497	−4.20	103	$7/2^+$	−0.493	−0.347	−0.018	−3.88	−3.4(17)
						109	$1/2^-$	−0.498	−3.78	0.007	−0.431	−0.41274(29)
$_{55}$Cs	$6s_{1/2}$	133	$7/2^+$	−0.716	−0.209	131	$5/2^+$	−0.716	−0.596	−0.001	0.389	0.45(5)[a]
						135	$7/2^+$	−0.716	−0.247	0.002	0.039	0.037(9)[b]
						134	4^+	−0.716	−0.371	0.000	0.163	0.169(30)
$_{56}$Ba$^+$	$6s_{1/2}$	135	$3/2^+$	−0.747	−1.03	137	$3/2^+$	−0.747	−1.03	0.001	0.001	−0.191(5)

Roberts and Ginges, PRA (2021)

Expt. data from: Persson, At. Data Nucl. Data Tables (2013)

Bohr-Weisskopf effect

From H-like experiments to heavy atom calculations

Accurate empirical BW effect from H-like ion measurements,

$$\mathcal{A}^{1\mathrm{s}}_{\mathrm{expt}} = \mathcal{A}^{1s}_{0}(1+\epsilon^{1s}) + \delta\mathcal{A}^{1s}_{\mathrm{QED}}\,.$$

BW effect with $\sim 1\%$ precision from measurements with H-like ^{203,205}Tl, ^{207}Pb, ^{209}Bi.

H-like ion result may be used to determine the BW effect in many-electron atoms!

$$\mathcal{A} = \mathcal{A}_0(1 + x_{\mathrm{scr}}\,\epsilon^{1s}) + \delta\mathcal{A}_{\mathrm{QED}}$$

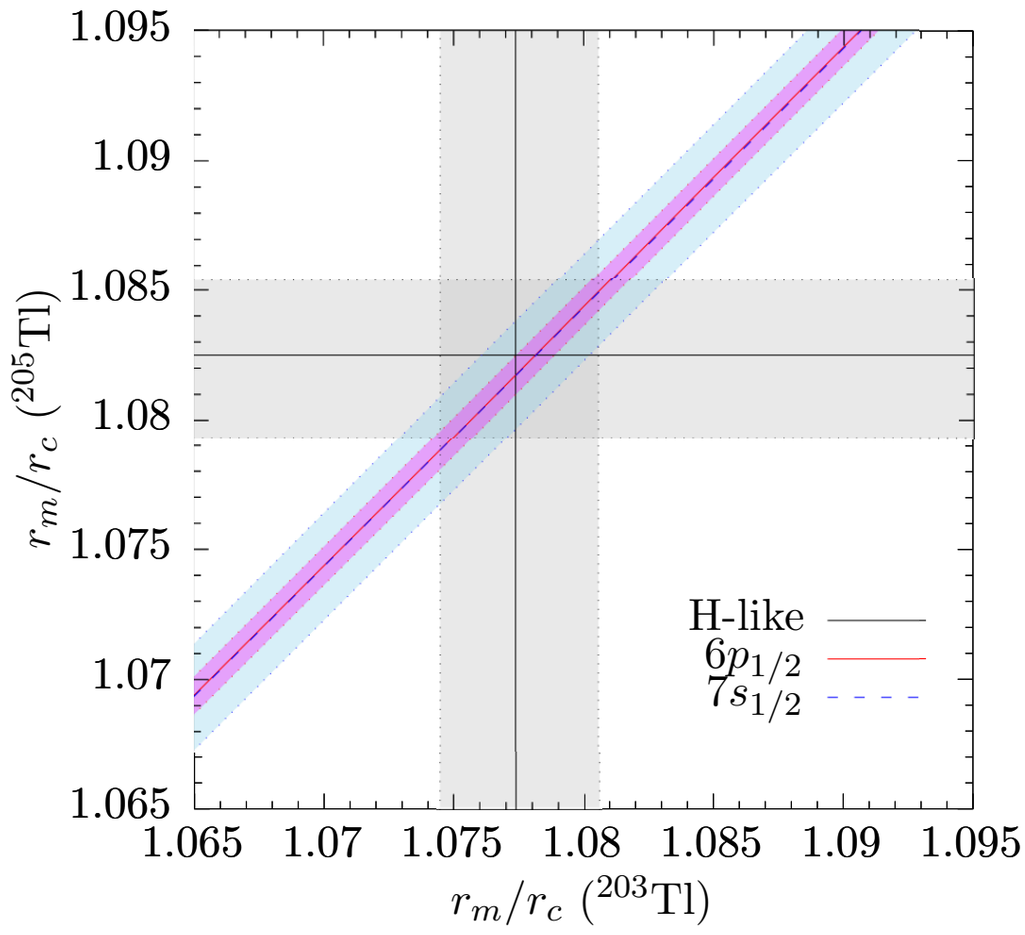
↑

electronic screening factor

For *s* states, $x_{\mathrm{scr}} \approx 1$, the uncertainty is negligible, and x_{scr} *is independent of the nuclear model!*

Nuclear structure uncertainty is entirely removed from atomic calculations!

Magnetization radius from H-like ion BW effect and neutral atom differential anomaly



Roberts and Ginges, PRA (2022)

Summary

Accurate modelling of the finite magnetization distribution in atomic nuclei is important for

- Hyperfine comparisons
  - Tests of atomic wave functions in the nuclear region
  - Reducing APV theory uncertainty to 0.1%
- Nuclear structure theory
- Determination of nuclear moments
- Probing the neutron distribution
- Tests of quantum electrodynamics