Study of electric dipole amplitudes for alkali-like atoms and implications for atomic parity violation

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High-precision study of E1 transitions

High-precision calculations

- E1 amplitudes for s, p, d transitions
- K, Ca^+, Rb, Sr^+, Cs, Ba^+, Fr, Ra^+ (and Li, Be^+, Na, Mg^+)
- 14 E1 transitions each – well over 100

High-precision calculations

- 46 high-precision experimental amplitudes
  - Also compiled large number other theory calculations
- Allows statistical analysis
- Test theory **and** test uncertainty method

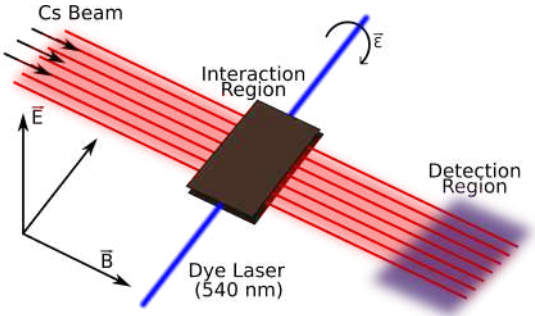
Motivation

- Tests of atomic theory for atomic parity violation
- Recent high-precision measurements in alkali and alkali-likes
- Development of atomic clocks

Motivation: PNC

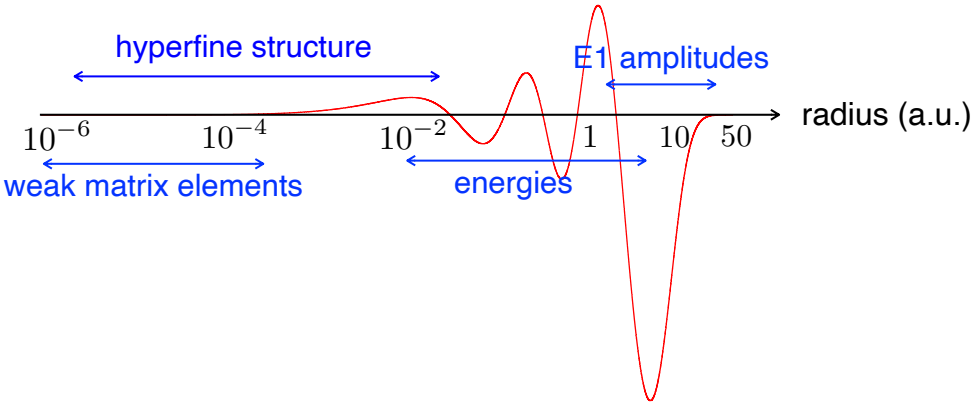
Atomic Parity Violation

- Currently: theory-limited
- PNC – chasing ∼0.1% accuracy
- Need accurate calculations, AND:
- Crucial to confidently determine theoretical accuracy
- Jens Erler talk: currently an issue!



Motivation: Probing wavefunctions

$$E_{\mathrm{PNC,z}} = \sum_n \frac{\langle a|d_z|n\rangle\langle n|h_W|b\rangle}{E_b - E_n} + c.c$$



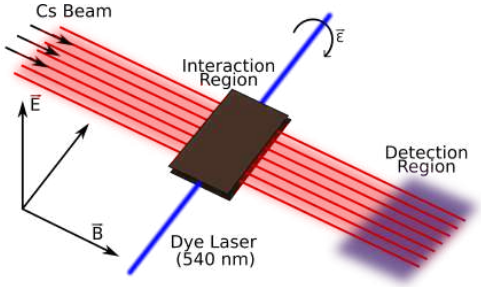
See: Jacinda's talk re: hyperfine

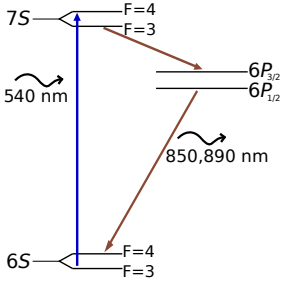
Motivation: $6S - 7S$ vector transition polarisability, β

Stark interference: – See Dan Elliott's talk!

$$A_{6S-7S} = A_{\mathrm{pnc}} + A_{\mathrm{stark}} + A_{M1}$$

$$A_{\mathrm{stark}} \sim \alpha E_{zz} + \beta E_{\perp} \quad \text{[Bouchiat, Bouchiat J. de Phys. 36 493 (1975)]}$$





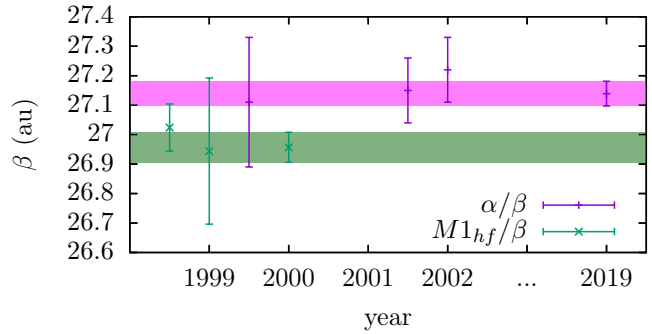
$$\mathrm{Im}(A_{\mathrm{PNC}})/\beta_{\mathrm{stark}} = 1.5935(56)\,\mathrm{mV/cm}$$

Wood *et al.*, Science **275**, 1759 (1997).

Motivation: $6S - 7S$ vector transition polarisability, β

- Currently 2.8σ discrepancy between β derived via two methods
- Both methods should be highly accurate

- Talks by Dan Elliott and Andrei Derevianko



All come from single experiment: *New α/β measurement planned @ Perdue – Elliott

- $\alpha/\beta = 9.905(11)$ – Cho, Wood, Bennett, Roberts, Wieman Phys. Rev. A **55**, 1007 (1997)
- $M1_{hf}/\beta = -5.6195(91)$ V/cm – Bennett, Wieman Phys. Rev. Lett. **82**, 2484 (1999)

Motivation: β (references)

Measurements:

- $M1_{hf}/\beta = -5.6195(91)$ V/cm – Bennett, Wieman Phys. Rev. Lett. **82**, 2484 (1999)
- $\alpha/\beta = 9.905(11)$ – Cho, Wood, Bennett, J. Roberts, Wieman Phys. Rev. A **55**, 1007 (1997)

Interpretations:

Calculation of α (theory + expt.)

- Safronova *et al.*, PRA**60**, 4476 (1999)
- Vasilyev *et al.*, PRA**66**, 020101 (2002)
- Dzuba *et al.*, PRD**66**, 076013 (2002)
- Toh *et al.*, PRL**123**, 073002 (2019)
- Sahoo *et al.*, PRD**103**, 111303 (2021)

Ab-initio calculation of $M1_{\mathrm{hf}}$

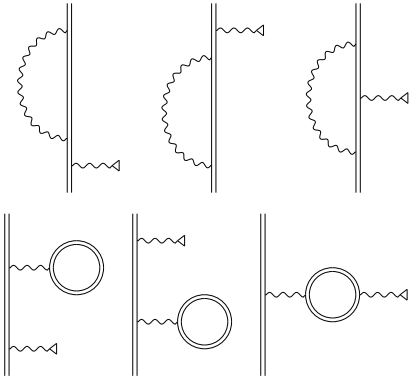
- Derevianko *et al.*, PRA**60**, 1741 (1999)

Semi-empirical calculation of $M1_{\mathrm{hf}}$

- Bennett, Weiman, PRL**82**, 073002 ('99); Bouchiat Piketty JPB**49**, 1851 ('88)
- Dzuba, Flambaum, PRA**62**, 052101 (2000)

Motivation: QED

- QED corrections to to E1 amplitudes
- Known to be important for very light atoms
- Precision for heavy single-valence systems:
  - Important here also!



QED Corrections

- Self-energy: non-local + difficult
- Rigorous QED in simplified atomic potentials
- OR, Approximate QED with many-body atomic physics

Radiative potential method

- Approximates self-energy with local potential
- Vertex cannot be included
- (Uehling vertex simple to calculate: completely negligible)

- Flambaum, Ginges, PRA**72**, 052115 (2005)

- Talks by Victor Flambaum, Jacinda Ginges

Motivation: QED + many-body

Atom	$\lvert r_{ab}\rvert$	This work		Sapirstein and Cheng [7]		
		PO(s)	PO(p)	PO(s)	PO(p)	vertex[a]
Na	4.588	0.032	0.000	0.031	0.001	-0.015
K	5.681	0.069	0.000	0.067	0.000	-0.003
Rb	6.009	0.190	0.000	0.182	0.000	0.028
Cs	6.585	0.334	-0.001	0.326	0.000	-0.065
Fr	6.511	0.777	-0.014	0.787	0.202	-0.060

[a] Vertex and other corrections. A full breakdown of these contributions is given in Table II of Ref. [7].

- Many-body effects significantly larger than disagreement
  - In particular: relaxation
- $\sim$20% for s-p; Changes sign and order-of-magnitude for p-d
- QED correction to s-states in core

• PhD student: Carter Fairhall [to be published soon]

Sapirstein, Cheng, PRA**71**, 022503 (2005); BMR, Dzuba, Flambaum, PRA**87**, 054502 (2013).

Caveat/Warning

- Method works well for energies and E1 amplitudes
- However: not always appropriate
- Missed (vertex) effects can be large and dominate
- e.g., Hyperfine constant, PNC matrix elements
- Incorrect sign and order-of-magnitude

- Flambaum, Ginges, PRA**72**, 052115 (2005)
- BMR, Dzuba, Flambaum, PRA**87**, 054502 (2013)
- BMR, Ginges, PRD**105**, 018301 (2022)

Motivation: QED

Several cases: QED *larger* than discrepancy between theory + experiment(!)

a	b	δ_{QED}	Theory	Expt.	Δ	Δ(%)
			Rb			
$5s_{1/2}$	$5p_{1/2}$	0.0019	4.2381	4.231(3)[1]	0.007	0.1
	$6p_{1/2}$	**-0.0012**	0.3232	0.3235(9)[2]	-0.0003	-0.1[†]
	$5p_{3/2}$	0.0027	5.9818	5.978(5)[1]	0.004	0.06[†]
	$6p_{3/2}$	-0.0015	0.5256	0.5230(8)[2]	0.0026	0.5
			Cs			
$6s_{1/2}$	$6p_{1/2}$	**0.0034**	4.5052	4.5057(16)[3]	-0.0005	-0.01[†]
	$7p_{1/2}$	**-0.0023**	0.2776	0.2781(4)[4]	-0.0005	-0.2
	$6p_{3/2}$	**0.0051**	6.3402	6.3398(22)[3]	0.0004	0.01[†]
	$7p_{3/2}$	**-0.0026**	0.5741	0.5742(6)[4]	-0.0001	-0.01[†]

- PhD student: Carter Fairhall

1. Volz and Schmoranzer, Phys. Scr. **T65**, 48 (1996).
2. Herold, Vaidya, Li, Rolston, Porto, Safronova Phys. Rev. Lett. **109**, 243003 (2012)
3. Toh, Damitz, Tanner, Johnson, Elliott Phys. Rev. Lett. **123**, 073002 (2019)
4. Damitz, Toh, Putney, Tanner, Elliott Phys. Rev. A **99**, 062510 (2019)

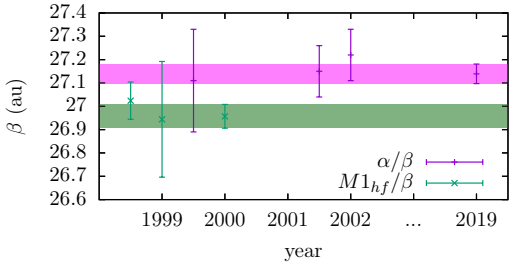
Require: Robust method for theoretical uncertainties

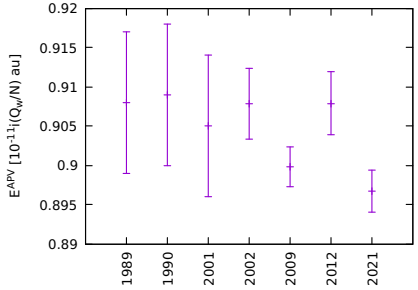
Extremely important

- Robust method for reliably determining theoretical uncertainties
- 0.5% $\rightarrow$ 0.1% level: requires proof
- Proving accuracy at this level is not simple task

Benchmarking atomic theory

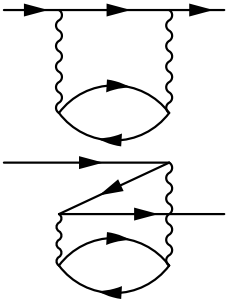
- Test h_{PV} with hyperfine
  - Nuclear uncertainties 0.5% – 0.2% level
  - Jacinda's talk
- Test E1
  - Limited by experiment (in some cases)
- Effects non-linear in $\boldsymbol{d}$ and h_{PV} ??
- Even numerical errors significant at this level





Outline of method

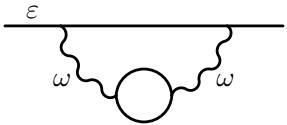
Goldstone:



$$\sum_{amn} \frac{g_{vamn} g_{nmav}}{\varepsilon_v + \varepsilon_a - \varepsilon_m - \varepsilon_n}$$

$$\sum_{abn} \frac{g_{vnba} g_{banv}}{\varepsilon_v + \varepsilon_n - \varepsilon_a - \varepsilon_b}$$

Feynman:



$$\int \frac{d\omega}{2\pi} G(\varepsilon + \omega) Q \Pi(\omega) Q$$

Vladimir Dzuba talk

• Dzuba, Flambaum, Silvestrov, Sushkov, Physics Letters A **131**, 461 (1988); Dzuba, Flambaum, Sushkov, Physics Letters A **140**, 493 (1989); Dzuba, Flambaum, Kraftmakher, Sushkov, Physics Letters A **142**, 373 (1989).

Beyond second-order

Coupled cluster:

- Expand wavefunction to fixed (finite) order of excitations from reference
- Solve iteratively for expansion coefficients: all-orders (in Coulomb interaction)
  - Talks by Sahoo, Chakraborty, Derevianko

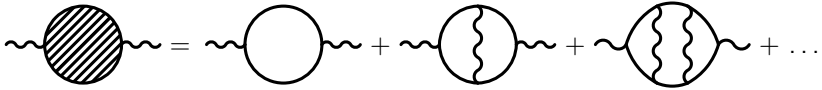
Feynman technique:

- Dominating series of screening diagrams summed exactly to all-orders
- all-orders in screening + hole-particle (double, triple, quadupole etc. excitations)
- No basis required, instead integration over frequencies
- Highly accurate, highly computationally efficient
  - Talks by Dzuba, Flambaum

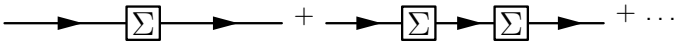
• Dzuba, Flambaum, Silvestrov, Sushkov, Physics Letters A **131**, 461 (1988); Dzuba, Flambaum, Sushkov, Physics Letters A **140**, 493 (1989); Dzuba, Flambaum, Kraftmakher, Sushkov, Physics Letters A **142**, 373 (1989).

Screening + Hole-particle + chaining

$$Q^{\mathrm{scr.}}(\omega) = Q + Q(-i\Pi Q) + +Q(-i\Pi Q)^2 + \ldots$$
$$= Q\left[1 + i\Pi(\omega)\right]^{-1}$$



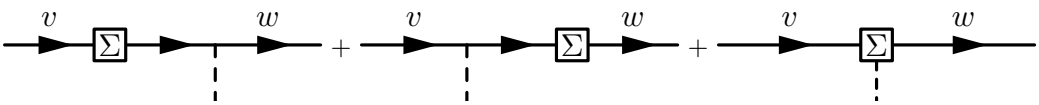
$$V_0^a = y_{aa}^0(r) - \sum_{k=2}^{\mathrm{even}} \frac{|\langle a||C^k||a\rangle|^2}{(2j_a+1)^2} y_{aa}^k(r)$$



$$(H + \Sigma(\varepsilon) - \varepsilon)\,\phi = 0$$

See also Vladimir Dzuba talk

SR + Norm (non-Brueckner)



Structure Radiation:

- Non-separable Σ and h_{external}
- $< 1\%$

Normalisation:

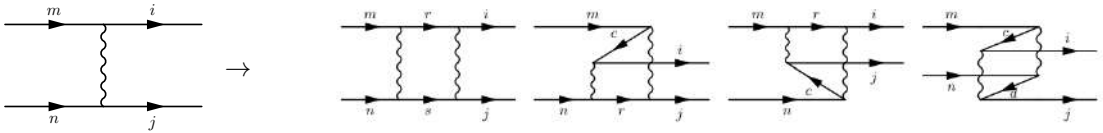
- Change in normalisation of many-body states

- Goldstone technique (direct diagram calculation)
- Only computationally intensive part (still $\sim$ minutes)
- Easily saturate basis

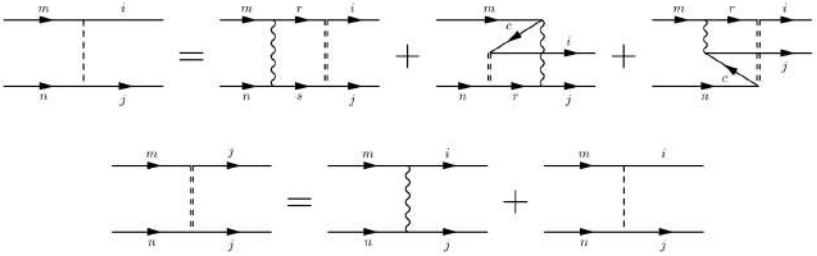
Johnson, Idrees, Sapirstein, PRA**35**, 3218 (1987); Dzuba, Flambaum, Silvestrov, Sushkov, J. Phys. B **20**, 1399 (1987)

Missing: ladder diagrams

Lowest (third) order:



All orders:



Similar to: Dzuba, PRA **78**, 042502 (2008)

Ladder diagrams [preliminary]

Table: Ab initio calculations of ionization energies (cm^{-1}) for the lowest states of Cs.

Level	RHF	$\delta\Sigma^{(2)}$	$\delta\Sigma^{(\infty)}$	Breit	QED	Final	Expt.	Δ(%)
$6s_{1/2}$	27954	4458	-998	2.8	-21.5	31395	31406	-0.04%
$6p_{1/2}$	18791	1747	-294	-7.4	1.1	20236	20228	0.04%
$6p_{3/2}$	18389	1550	-258	-0.7	0.1	19680	19674	0.03%
$5d_{3/2}$	14138	3424	-458	25.8	5.6	17136	16907	1%
$5d_{5/2}$	14163	3240	-402	30.3	4.7	17035	16810	1%

Table: Ladder corrections to the lowest d-state energies of Cs, showing the lowest (third-order) $\delta L^{(3)}$ and subsequent all-order $\delta L^{(\infty)}$ corrections (including chaining). The column Σ is the all-orders correlation potential result including Breit and QED

Level	Expt.	Σ	Δ(%)	$\delta L^{(3)}$	$\delta L^{(\infty)}$	Total	Δ(%)
$5d_{3/2}$	16907	17136	1%	-173	-60	16903	-0.03%
$5d_{5/2}$	16810	17035	1%	-175	-64	16796	-0.08%

Similar to: Dzuba, PRA **78**, 042502 (2008)

Estimate higher-order diagrams + uncertainty

Re-scale Σ to match experimental energies:

$$\Sigma \to \lambda\Sigma$$

- $\lambda \approx 1$
- Enter at $\sim 0.05\%$ level (for s-p)
- $\sim 0.5\%$ level (for p-d)
- Must account for QED, Breit (no double-counting)

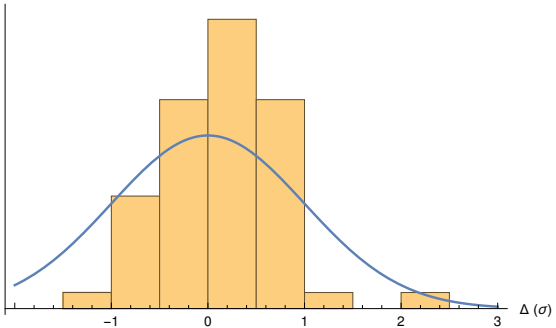
Estimate uncertainty:

- Compare $\lambda\Sigma^{(2)}$, $\Sigma^{(\infty)}$, $\lambda\Sigma^{(\infty)}$
- $\sim$30% From Breit, QED, SR+Norm
- Uncertainty: always larger than $\delta\lambda$ semi-empirical correction

Overview: E1 calculations

Consider large number of transitions

- K, Ca^+, Rb, Sr^+, Cs, Ba^+, Fr, Ra^+
- Exact same method + parameters
- 14 E1 transitions each – over 100
- 46 high-precision experimental amplitudes
- Allows statistical analysis:
  - Thorough test of the theory accuracy
  - **Test of method for uncertainty estimation**

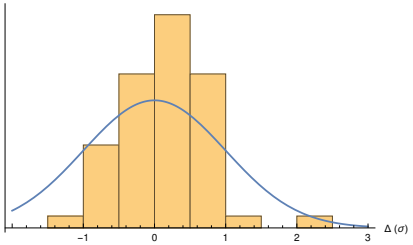


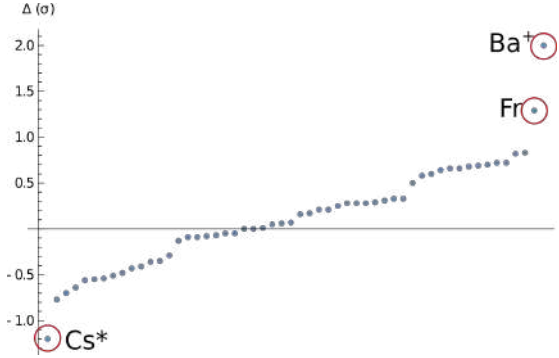
- Also did Li, Be^+, Na, Mg^+
- Agreement (unsurprisingly) excellent, not included in analysis (too simple)

Results: Overview

Compared with 46 high-precision experiment

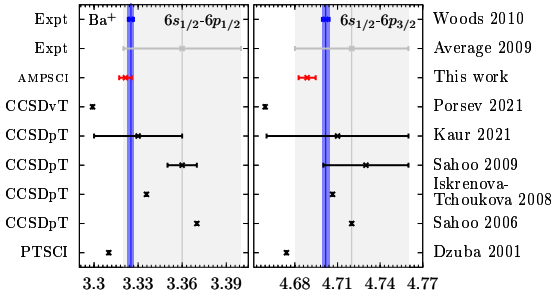
- All but 2 (or 3) within 1σ
  - Combined theory+experiment errors
  - Dominated by theory (mostly)
- Better than statistically expected
  - Conservative uncertainties!
- $\approx$ Half within experimental uncertainties!
  - Require experimental improvements

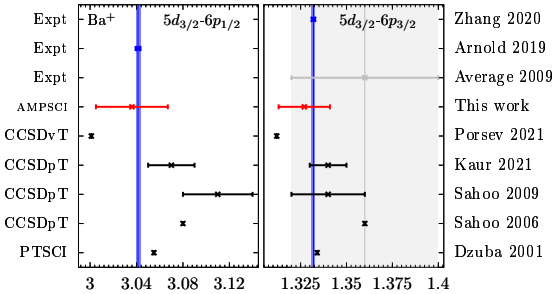




- Cs case (single transition): return later

Ba^+





- Largely agree, though large spread in theory – some disagree very significantly
  - Highlights importance of robust theory uncertainty estimate
- Largest disagreement: $6s$-$6p_{3/2}$ (2σ)
- While single 2σ in ~ 46 cases is expected, we think this may be experimental issue

Reduced matrix elements $|\langle a||d||b\rangle|$ (ea_0) – See arXiv:2211.11134 for full references

Ba^+: Ratio

Also 2σ tension in ratio

$$\frac{|\langle 6s||d||6p_{3/2}\rangle|}{|\langle 6s||d||6p_{1/2}\rangle|} = \begin{cases} 1.4116(2) & \text{Theory} \\ 1.4140(12) & \text{Expt. [Woods } et\ al\text{, PRA (2010)].} \end{cases} \tag{1}$$

c.f. Rb (for example) – Ba^+ difference is 100x larger!

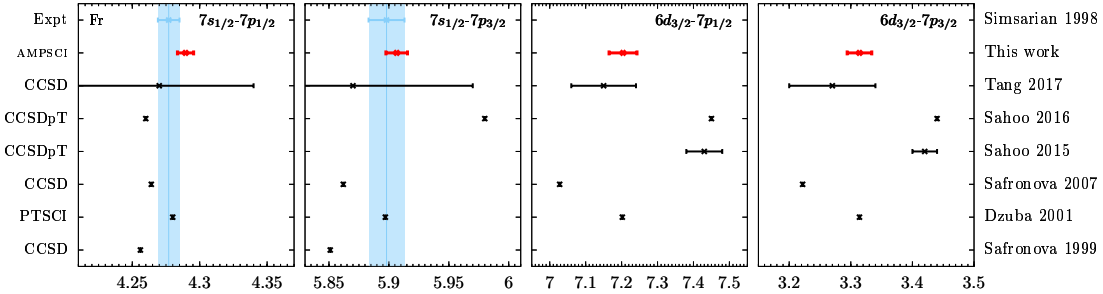
$$\frac{|\langle 5s||d||5p_{3/2}\rangle|}{|\langle 5s||d||5p_{1/2}\rangle|} = \begin{cases} 1.41141(9) & \text{Theory} \\ 1.41144(1) & \text{Expt. [Leonard } et\ al\text{, PRA (2015)].} \end{cases} \tag{2}$$

Correlations cancel. Non-rel limit: $\sqrt{2} = 1.41421$

Other theory*:

- 1.4109(2) – Iskrenova-Tchoukova *et al.* (2008)
- *1.412 – Dzuba* et al. *(2001)*
- *1.40 – Sahoo* et al. *(2006)*
- *1.411 – Kaur* et al. *(2021),*
- *1.412 – Porsev* et al. *(2021)*

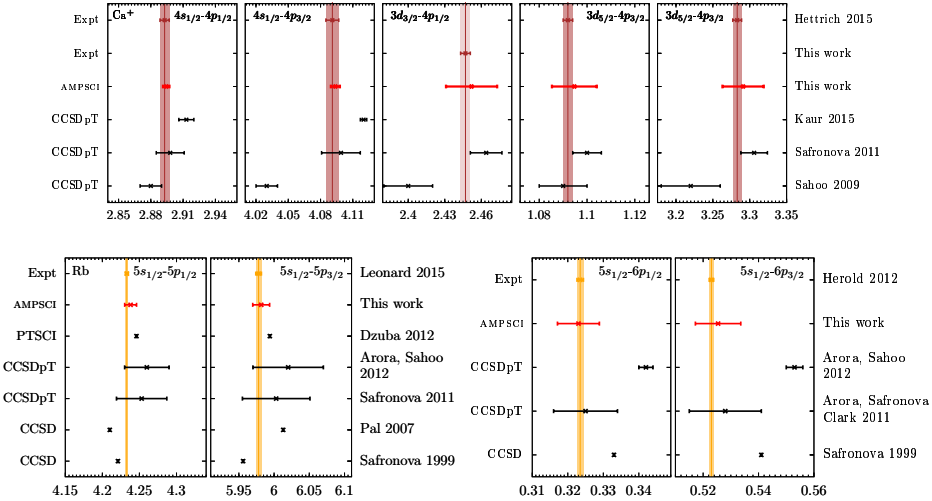
Fr



- Other discrepancy: Fr $7s$-$7p_{1/2}$ - 1.2σ – within expectations
- Large spread in theory values, limited experiment
- Based on comparison for other systems: expect ours to be most accurate

Reduced matrix elements $|\langle a||d||b\rangle|$ (ea_0) – See arXiv:2211.11134 for full references

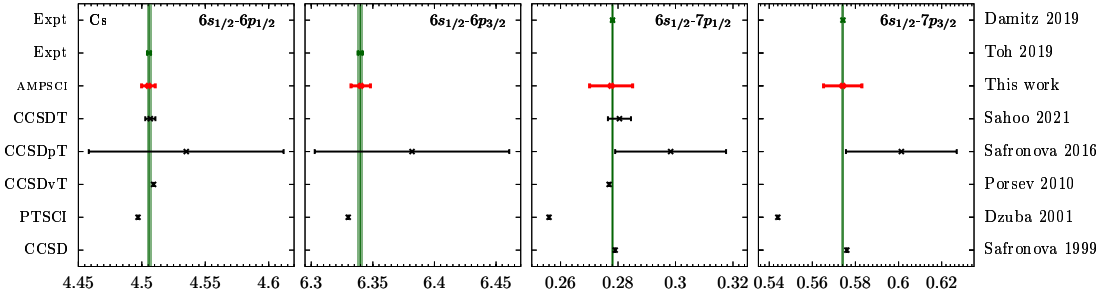
“Light” atoms: excellent agreement (no surprise)



Again, some theory strongly disagrees: highlights need to correct uncertainty analysis

Reduced matrix elements $|\langle a||d||b\rangle|$ (ea_0) – See arXiv:2211.11134 for full references

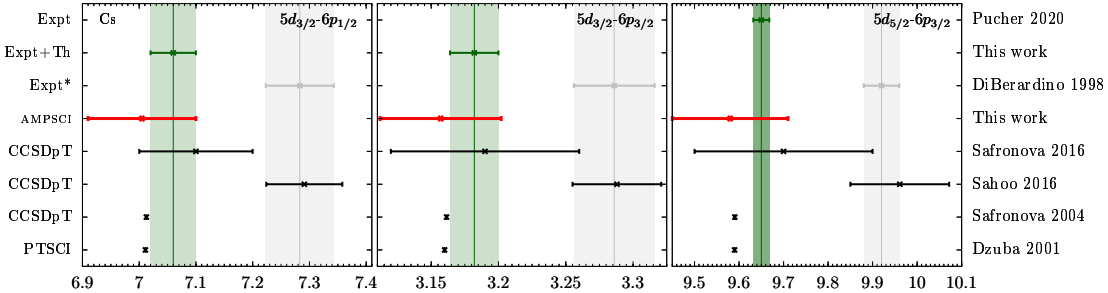
Results: Cs



- Most precise experiment is for Cs:
- Excellent agreement between theory and experiment for 6s-np
- Even for extremely small (6s-7p), small due to cancellations

Reduced matrix elements $|\langle a||d||b\rangle|$ (ea_0) – See arXiv:2211.11134 for full references

Results: Cs d-states



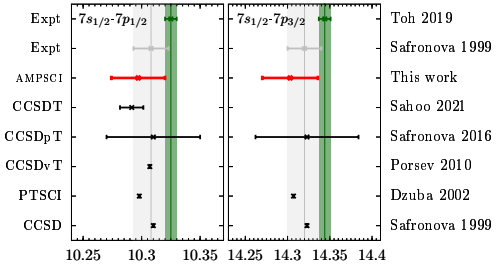
- New lifetime measurement
- Resolves discrepancy between theory and experiment (favour of theory)
- Much better agreement than expected for CP method
  - Dzuba, Flambaum, Ginges, PRA**63**, 062101 (2001).
  - Claimed 5% uncertainty for p-d: actually 0.5%!
- Highlights need for roust theory uncertainties

Pucher, Schneeweiss, Rauschenbeutel, Dareau, Phys. Rev. A **101**, 042510 (2020).

Important case: Cs $7s$–$7p$

Updated value

- Extracted from $6s - 7s$ stark shift [1]
- New value [2] shifts by $\sim 1.1\sigma$ cf. previous [3]
- "only" 0.2% shift
- Problem for uncertainty 0.3% / goal of 0.1%!



1. Bennett, J. L. Roberts, Wieman, PRA**59**, R16(R) (1999)
2. Toh, Damitz, Tanner, Johnson, Elliott PRL**123**, 073002 '19
3. Safronova, Johnson, Derevianko, PRA**60**, 4476 (1999)

$$E_{\mathrm{PNC}} = \frac{\langle 7s|d_z|6p_{1/2}\rangle\langle 6p_{1/2}|h_{\mathrm{W}}|6s\rangle}{E_{6s} - E_{6p_{1/2}}} + \frac{\langle 7s|h_{\mathrm{W}}|6p_{1/2}\rangle\langle 6p_{1/2}|d_z|6s\rangle}{E_{7s} - E_{6p_{1/2}}} + \frac{\langle 7s|d_z|7p_{1/2}\rangle\langle 7p_{1/2}|h_{\mathrm{W}}|6s\rangle}{E_{6s} - E_{7p_{1/2}}} + \ldots$$

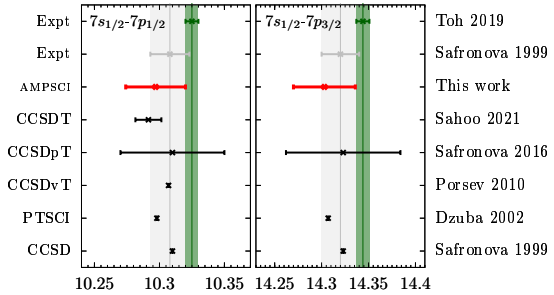
$$\approx -1.91 + 1.49 + 1.35 + \mathcal{O}(10^{-1})$$

- **Any shift in this ME leads directly to shift in** E_{PNC}

Important case: Cs $7s$–$7p$

Impact on PNC analysis

- $\sim 1.1\sigma$ disagreement; "only" 0.2% shift
- Compared to theory: actually $\sim$0.5% error!
- But leads directly to 0.5% shift in E_{PNC}
  - Nearly 2x claimed E_{PNC} uncertainty from *single term*
- Old value used in **all** uncertainty analyses!
- (Doesn't impact β issue)



- Issue with theory for $7s$ state?
- Issue with DC stark shift experiment?

Results: Extract new E1

Transition	$\lvert\langle a\rvert\rvert d\rvert\rvert b\rangle\rvert$	Method
	Cs	
$5d_{5/2}$–$5p_{3/2}$	9.650(18)	τ
$5d_{3/2}$–$6p_{1/2}$	$7.06(1)_{\mathrm{ex}}(4)_{\mathrm{th}}$	τ + Ratio
$5d_{3/2}$–$6p_{3/2}$	$3.182(6)_{\mathrm{ex}}(17)_{\mathrm{th}}$	τ + Ratio
$5d_{3/2}$–$7p_{3/2}$	0.795(4)	τ + E1 + Ratio
	0.799(5)	τ + E1 + Ratio
$5d_{5/2}$–$7p_{3/2}$	2.481(11)	τ + E1 + Ratio
	2.493(15)	τ + E1 + Ratio
	Fr	
$8s_{1/2}$–$7p_{1/2}$	4.234(20)	τ + Ratio
$8s_{1/2}$–$7p_{3/2}$	7.460(33)	τ + Ratio

Transition	$\lvert\langle a\rvert\rvert d\rvert\rvert b\rangle\rvert$	Method
	Ca^+	
$3d_{3/2}$–$4p_{1/2}$	2.447(4)	E1 + Ratio
	Sr^+	
$5s_{1/2}$–$5p_{1/2}$	3.076(24)	τ + Branching
$5s_{1/2}$–$5p_{3/2}$	4.360(23)	τ + Branching
$4d_{3/2}$–$5p_{1/2}$	3.093(15)	τ + Branching
$4d_{3/2}$–$5p_{3/2}$	1.378(34)	τ + Branching
$4d_{5/2}$–$5p_{3/2}$	4.175(22)	τ + Branching
	Ra^+	
$7s_{1/2}$–$7p_{1/2}$	3.229(9)	E1 + Ratio
$6d_{3/2}$–$7p_{1/2}$	3.564(27)	E1 + Ratio

See arXiv:2211.11134 for references

Summary

High-precision calculations

- E1 amplitudes for s, p, d transitions
- K, Ca^+, Rb, Sr^+, Cs, Ba^+, Fr, Ra^+

Uncertainty

- Compare to 46 high-precision experimental amplitudes
- Better than expected agreement: conservative uncertainty
- Half lie *within experimental errors*
- Many at 0.1% level or better: demonstrate robust uncertainty method

Also

- Extract several new E1 amplitudes from existing experiment

Upcoming postdoc position – UQ, Brisbane

- Funding for postdoc
- Know a great candidate?
- Not advertised yet, but put people in touch
- j.ginges @ uq.edu.au, b.roberts @ uq.edu.au