Atomic Parity Violation in Cs

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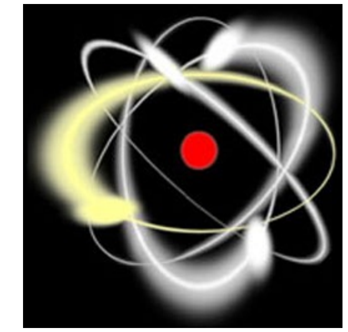
NSF

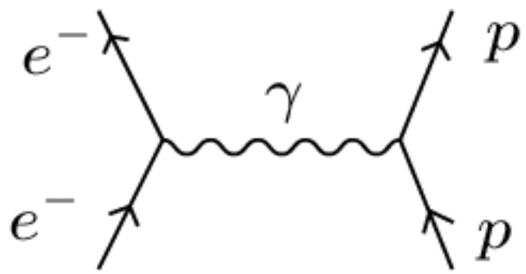
Atomic parity violation (APV)



Parity transformation: $\mathbf{r}_i \rightarrow -\mathbf{r}_i$

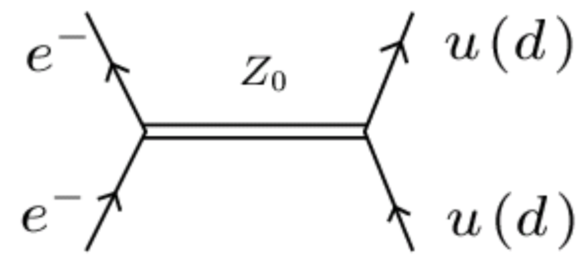
$[H_{atomic}, P]=0$ => Atomic stationary states are eigenstates of Parity

Electromagnetic



Conserve parity

Electroweak



Do not conserve parity

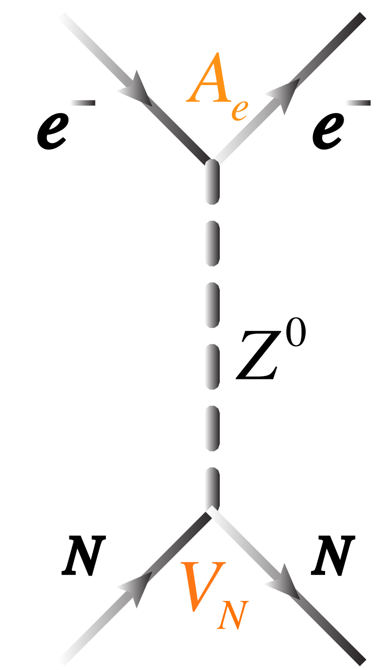
Z-boson exchange spoils parity conservation

What is the strength of electroweak coupling of quarks and electrons?

Wieman and Derevianko, arXiv:1904.00281
Safronova, Budker, DeMille, Kimball, Derevianko, & Clark, RMP 90, 25008 (2018)

Nuclear-spin independent effects

Electron axial-vector × nucleon vector current



Averaging over quarks - effective Hamiltonian in the electronic sector

$$H_W = Q_W \times \frac{G_F}{\sqrt{8}} \gamma_5 \rho_n(r)$$

weak charge

neutron distribution

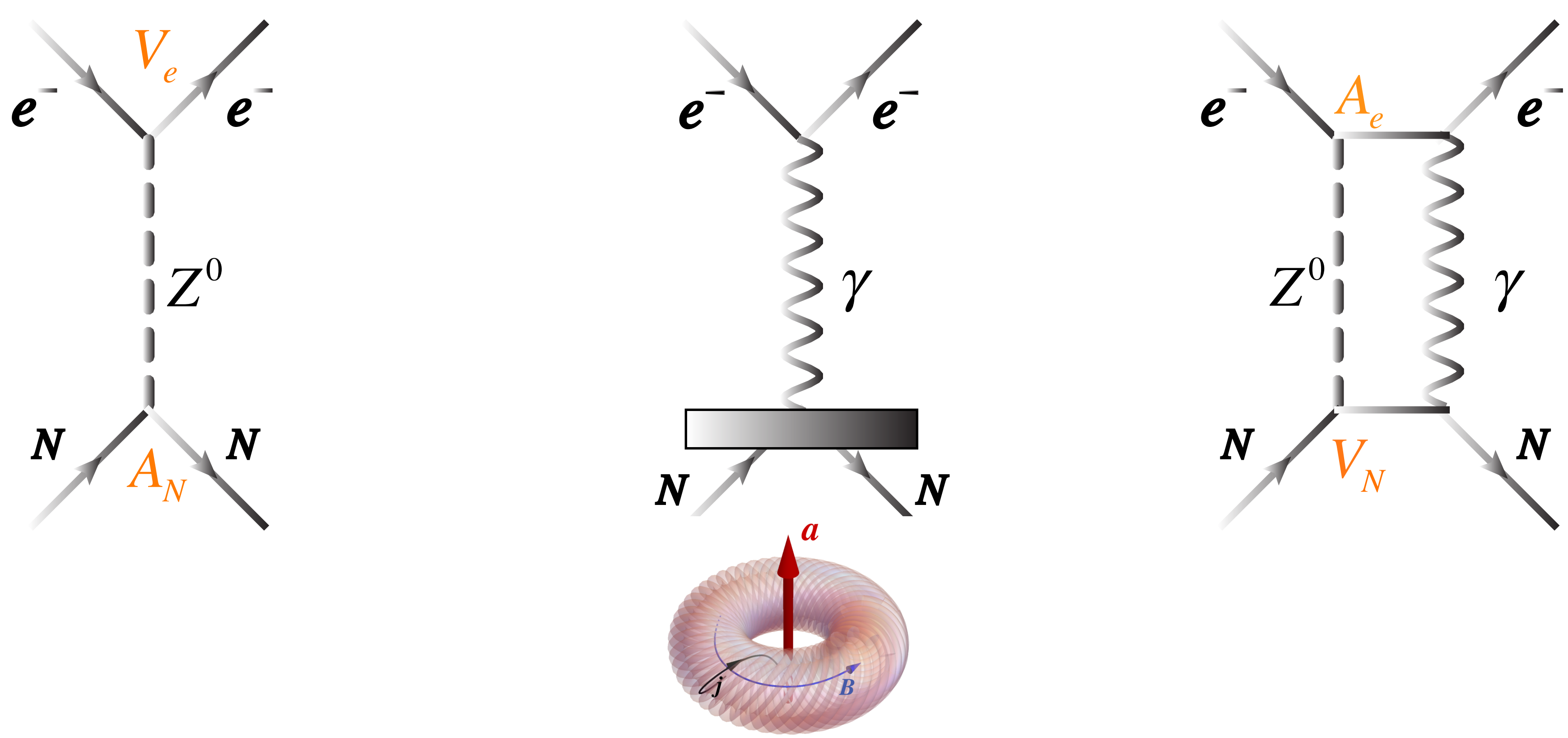
$$Q_W^{\mathrm{tree}} = -N + Z\left(1 - 4\sin^2\theta_W\right) \approx -N$$

Nuclear spin-dependent effects

For unpaired nucleon & open-shell atom

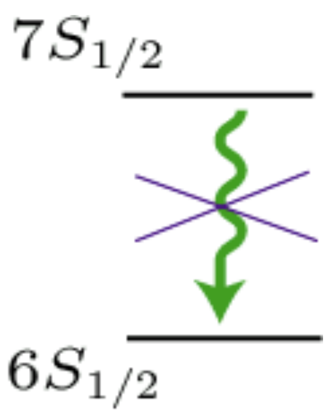
$$H_{\mathrm{NSD}} = \frac{G_F}{\sqrt{2}} \left(\eta_{\mathrm{axial}} + \eta_{\mathrm{anapole}} + \eta_{\mathrm{hyperfine}} \right) \boldsymbol{\alpha} \cdot \mathbf{I} \rho_n(r)$$

Nuclear spin



Nuclear anapole moment

Parity-violating 7S-6S amplitude in Cs

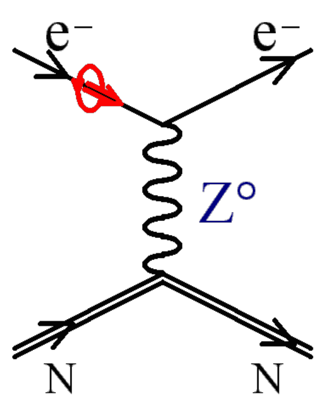


$$\langle 7S_{1/2} | D | 6S_{1/2} \rangle \equiv 0 \qquad D = \sum_{i=1}^{N} -e\,\mathbf{r}_i$$

Electric-dipole transition is forbidden by the **parity** selection rules

Weak interaction leads to an admixture of states of opposite parity

$$E_{\mathrm{PV}} = \overline{\langle 7S_{1/2}} | D | \overline{6S_{1/2} \rangle} \neq 0$$



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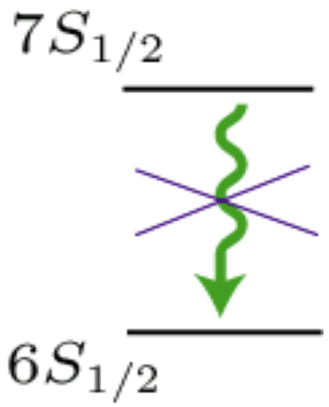

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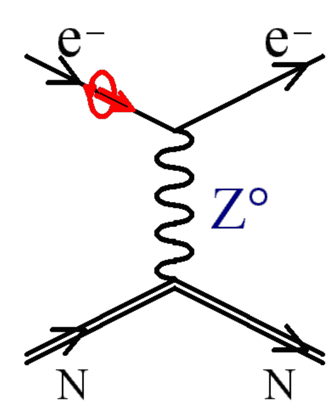
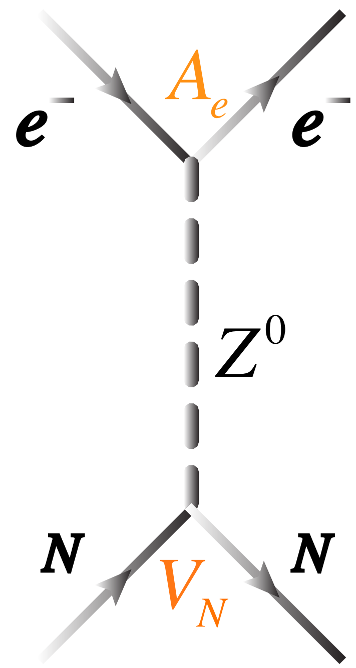


Tiny effect $E_{\mathrm{PV}} \sim 10^{-11}$ atomic units

Wieman and Derevianko, arXiv:1904.00281



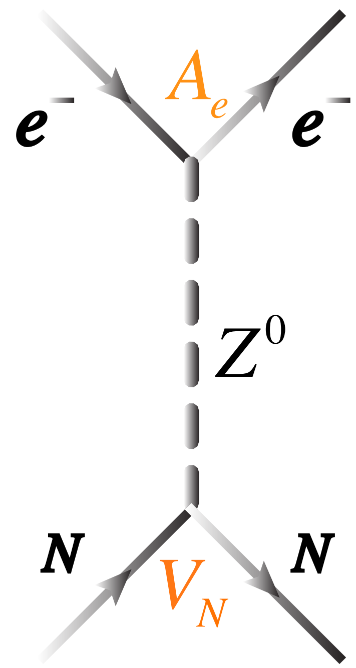
Weak charge extraction

$$H_W = Q_W \times \frac{G_F}{\sqrt{8}} \gamma_5 \rho_n(r)$$

Weak charge

neutron distribution

Weak charge extraction



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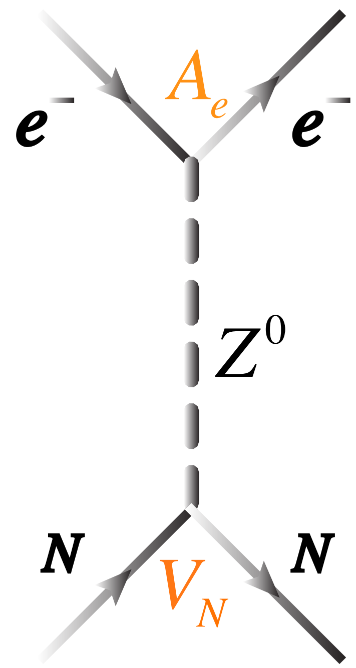
$$E_{PV} = k_{PV}\, Q_W$$

Weak charge extraction



$$H_W = Q_W \times \frac{G_F}{\sqrt{8}} \gamma_5 \rho_n(r)$$

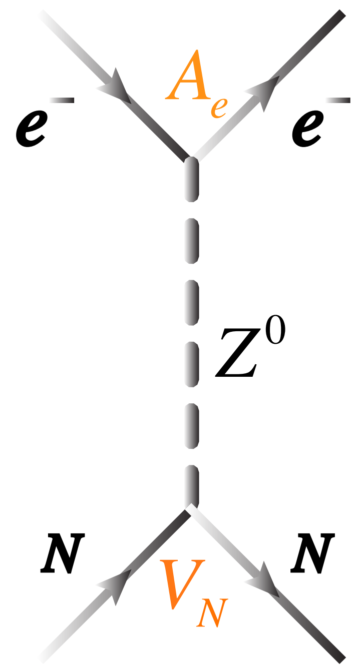
Weak charge

neutron distribution

$$E_{PV} = k_{PV} \, Q_W$$

measured

Weak charge extraction



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computed

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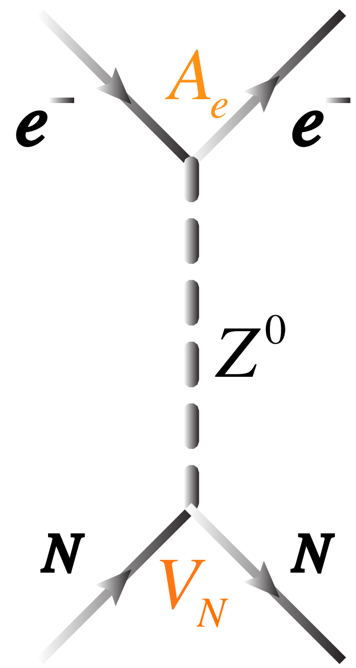

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Weak charge

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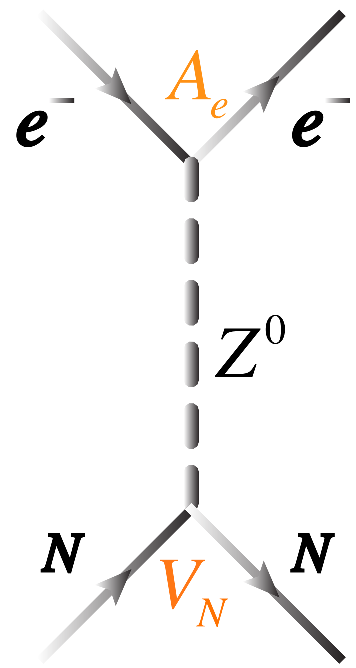
Signature of new physics:

$$Q_W^{\text{inferred}} = ? = Q_W^{\text{SM}}$$

Weak charge extraction



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Signature of new physics:

$$Q_W^{\mathrm{inferred}} = ? = Q_W^{\mathrm{SM}}$$

Two sources of uncertainties in Q_W: experimental (E_{PV}) and theoretical (k_{PV})

Weak charge of ^{133}Cs (as of 1999)

1997: measurement expt error 0.34% while theory (Notre Dame/Novosibirsk) error 1%

1999: Bennett & Wieman : reanalysis of the PV measurement+ reduction of theory error

$$\left.\begin{array}{ll}\text{Atomic Experiment} & E_{\text{PV}} \\ \text{Atomic Structure Theory} & E_{\text{PV}}/Q_W\end{array}\right\} \Rightarrow Q_W^{\text{inferred}} = -72.06(28)_{\text{expt}}(34)_{\text{theor}}$$

Standard Model $\quad Q_W^{\text{SM}} = -73.09(3)$

$$Q_W^{\text{inferred}} \neq Q_W^{\text{SM}}$$

2.5σ deviation (??? new physics, other corrections ???)

New physics scenarios:

extra *Z*-bosons, scalar leptoquarks, four-fermion contact interactions, etc

Experiment: Wood *et al*. (1997); Bennett and Wieman (1999) (Boulder group)
Theory: Dzuba, Sushkov, Flambaum (1989); Blundell, Johnson, and Sapirstein (1990).
SM calculations: Marciano and Rosner PRL (1990); Groom *et al* Eur. Phys. J (2000)

Weak charge of ^{133}Cs (as of 2005)

$$\sigma = 0.53\% \quad (\sigma_{expt} = 0.35\%, \sigma_{theor} = 0.4\%)$$

1999 Based on decade-old calculations by Dzuba *et al.* and Blundell *et al.*	2.5σ	Bennett & Wieman 1999
Breit interaction	-1.2σ	Derevianko (2000)
QED: Vacuum polarization (+ 0.8 σ) Vertex/self-energy (-1.3 σ)	-0.5σ	Johnson *et al.* (2002);Milstein & Sushkov (2002);Kuchiev & Flambaum (2002);Sapirstein *et al.* (2003);Shabaev *et al.* (2005)
Neutron skin	-0.4σ	Derevianko (2002)
Updated correlated value and vec. trans. polarizability	+0.7σ	Dzuba, Flambaum & Ginges (2002)
PV e-e, renormalization $q \to 0$, virtual exc. of the giant nuc. res.	-0.08 σ	Sushkov & Flambaum (1978) Milstein, Sushkov&Terekhov (2002)
Total deviation	1.0 σ	

Next step (2000-2010)

$$\sigma_Q = \sqrt{(\sigma_{\text{expt}})^2 + (\sigma_{\text{theor}})^2}$$

$$\sigma_{\text{expt}} = 0.35\% < \sigma_{\text{theor}} = 0.5\%$$

Theoretical uncertainty is limited by
the accuracy of solving
the basic correlation atomic-structure problem

Requirements to atomic-structure calculations

- Weak interaction occurs in the nucleus

$$\frac{v}{c} \sim \alpha Z \approx 0.5 \qquad \text{for Cs}$$

Ab initio relativistic calculations based on Dirac equation

- Calculations should have uncertainty better than 0.35%

Hartree-Fock calculations are off by 50% for important atomic properties

Many-body perturbation theory

Treat interaction beyond the Hartree-Fock as a perturbation

Our CCSDvT method

- ⇨ *Ab initio* relativistic many-body method
- ⇨ Based on coupled-cluster all-order scheme (additional inclusion of triple excitations + non-linear terms+…) CCSDvT
- ⇨ 1,000-fold increase in computational complexity over previous calculations (100 Mb → 100 Gb)
- ⇨ Code quality control: two persons + symbolic tools
- ⇨ Exact for 3e lithium: 0.01% accuracy demonstrated

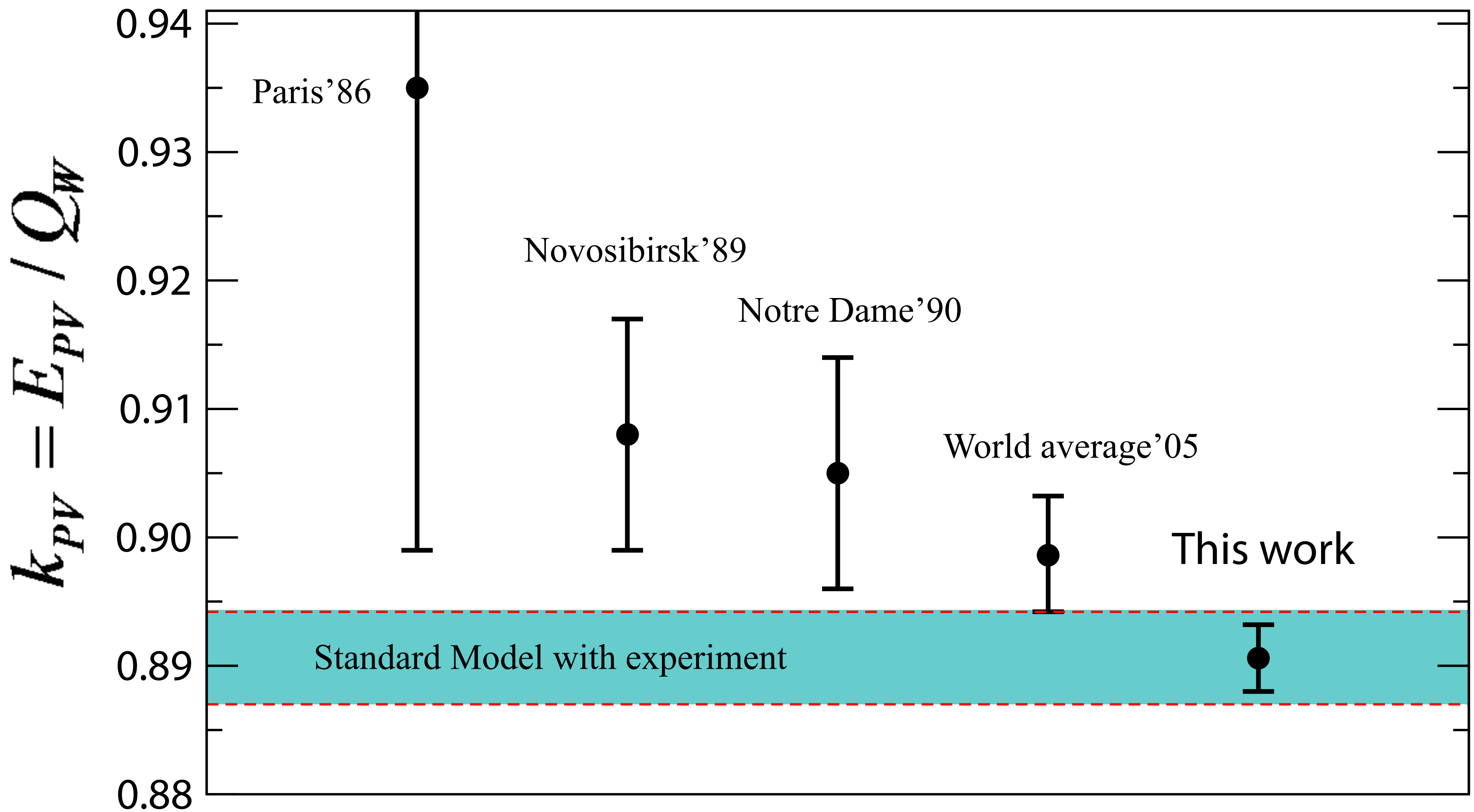
PV amplitude

$$E_{\rm PV} = \sum_n \frac{\langle 7S_{1/2} | D | nP_{1/2} \rangle \langle nP_{1/2} | H_W | 6S_{1/2} \rangle}{E_{6S} - E_{nP_{1/2}}} + \text{c.c.}(6S \leftrightarrow 7S)$$

$$H_W = Q_W \times \frac{G_F}{\sqrt{8}} \gamma_5 \rho_n(r)$$

Accuracy is important

Status as of 2010



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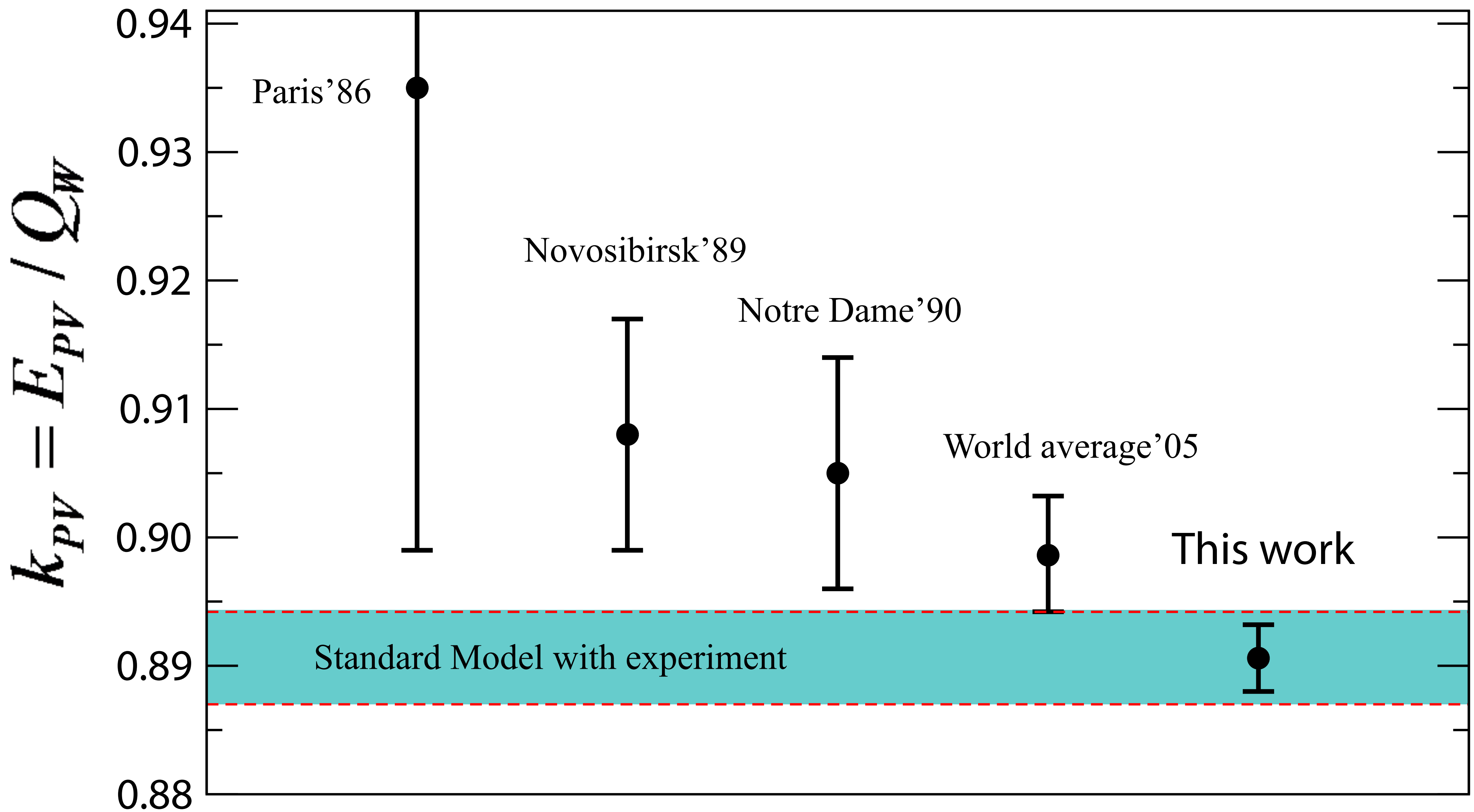
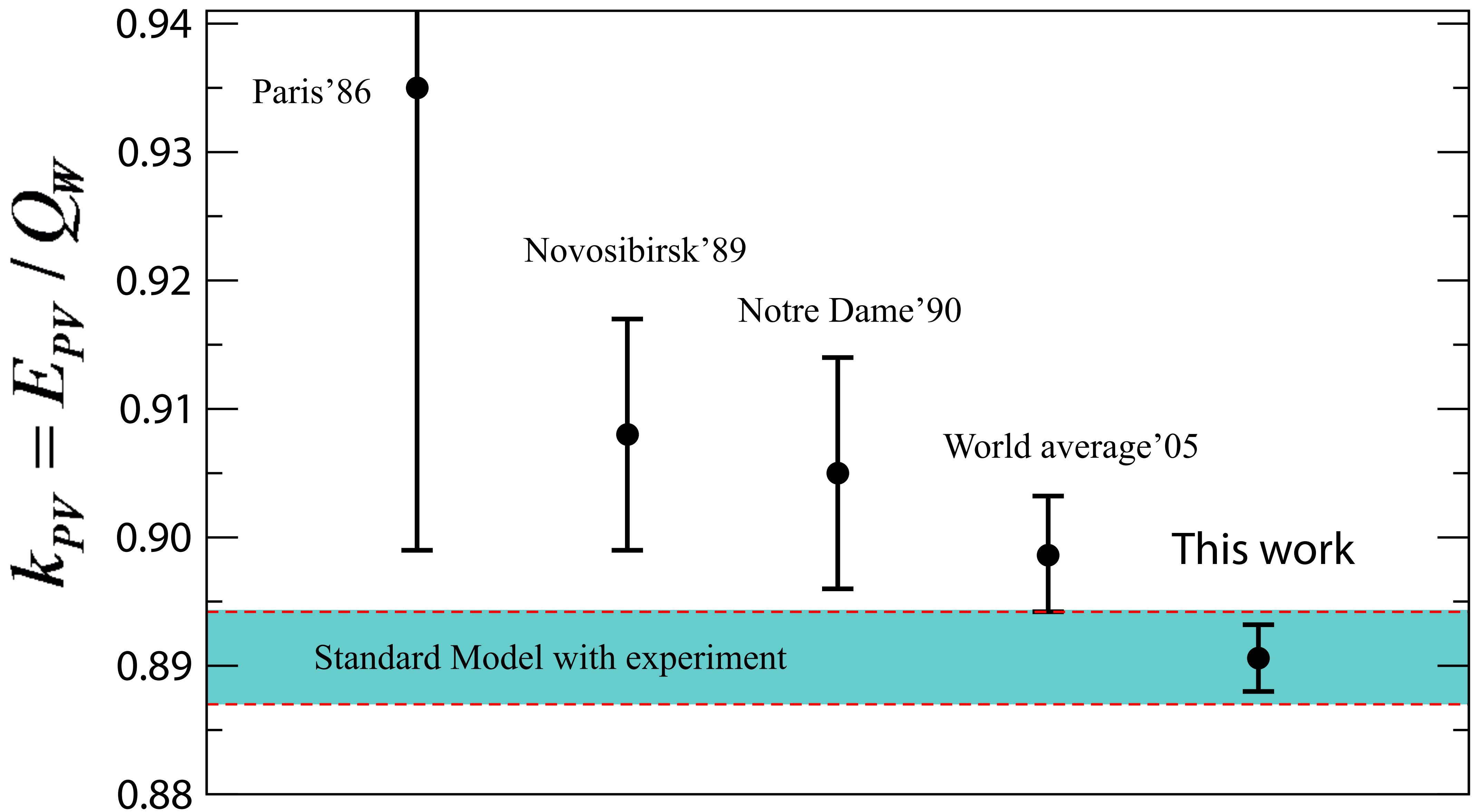


S. G. Porsev, K. Beloy and A. Derevianko, Phys. Rev. Lett. 102, 181601 (2009)
S. G. Porsev, K. Beloy and A. Derevianko, Phys. Rev. D 82, 036008 (2010)

Status as of 2010

Factor of two reduction in theoretical error + shift of the central value



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2020: Motivations to revisit APV in Cs

(1) Tension for the ^{133}Cs anapole moment with the nuclear theory
(2) Tension for supporting quantities (vector transition polarizability)
(3) More accurate experimental results for dipole matrix elements [Purdue]
(4) New experimental efforts on measuring APV in Cs [Purdue]
(5) Alternative to the sum-over state approach
(6) New dark-sector motivations

Di Xiao

Hoang Bao Tran Tan

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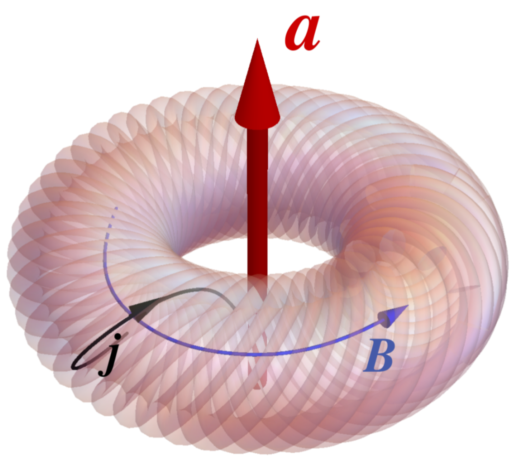
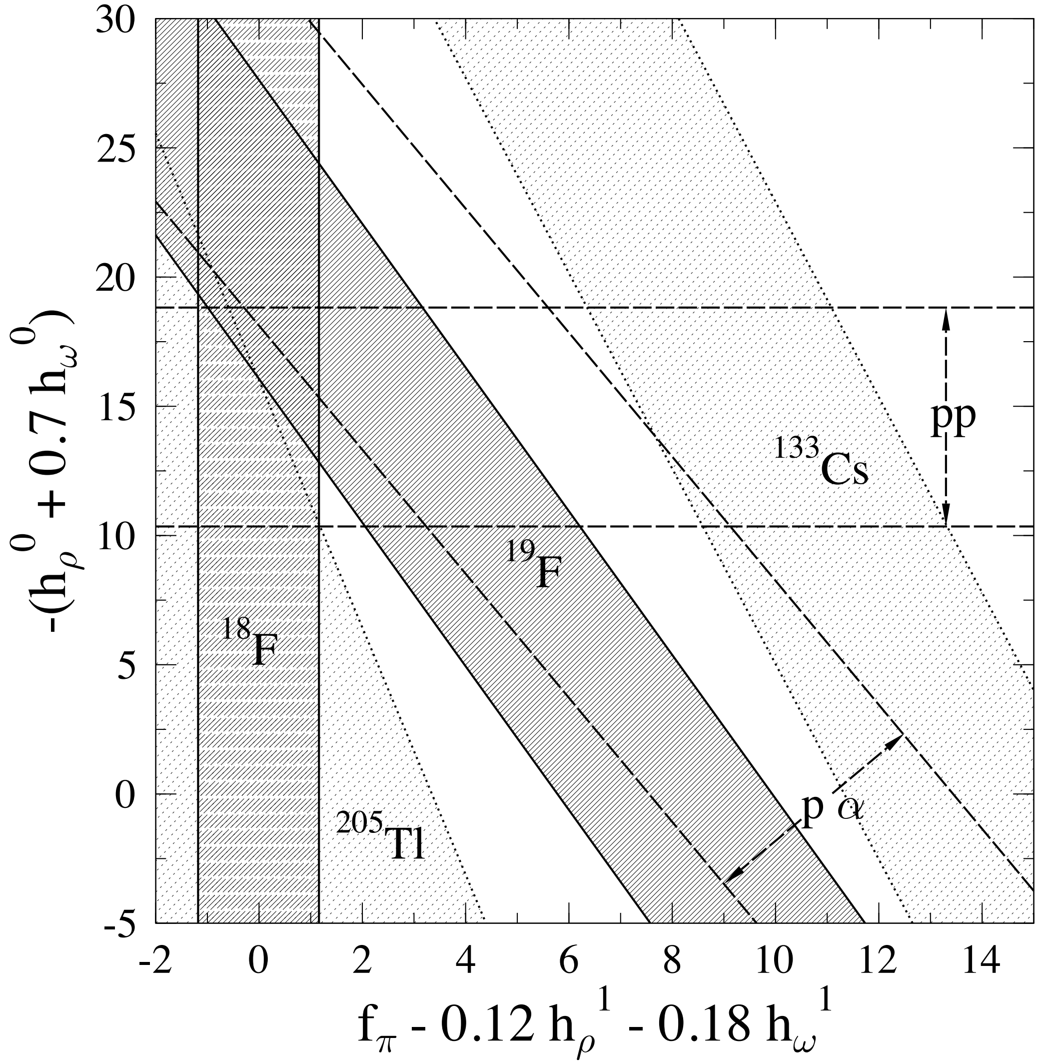
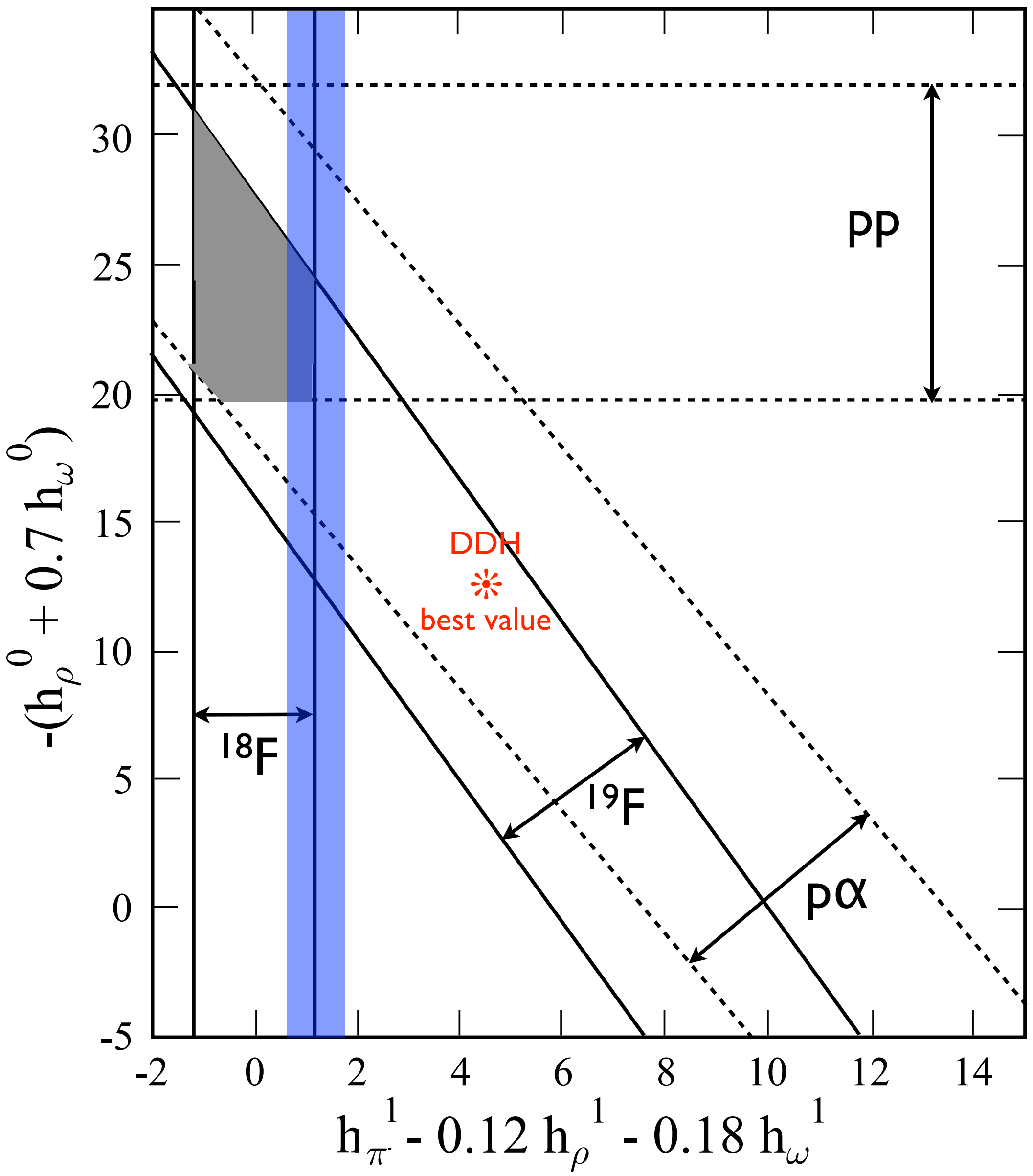


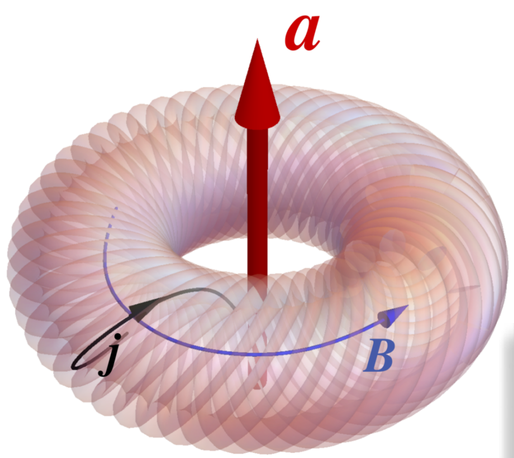
(1) Anapole tensions





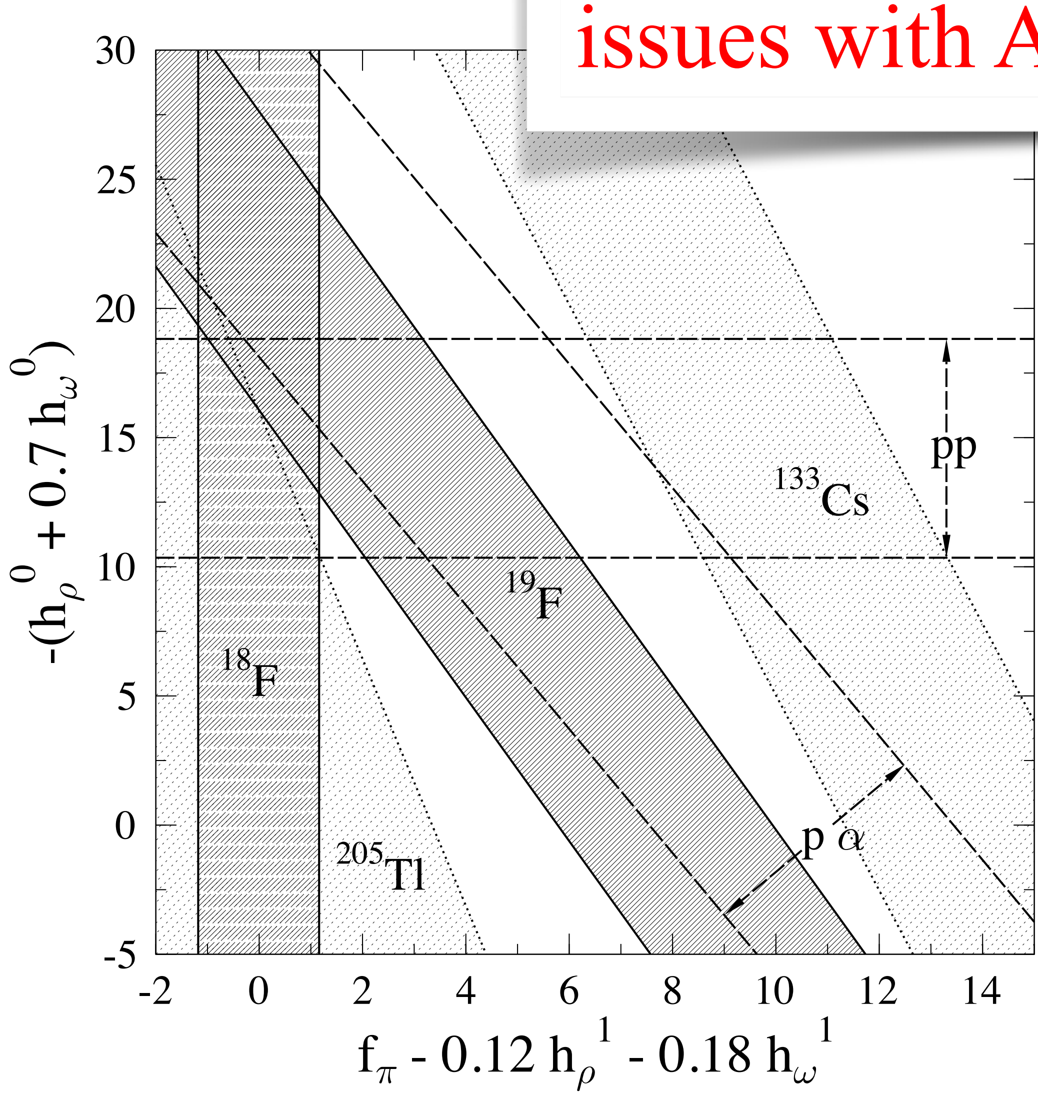
Haxton & Wieman
Ann. Rev. Nucl. Part. Sci. 51 261 (2001)

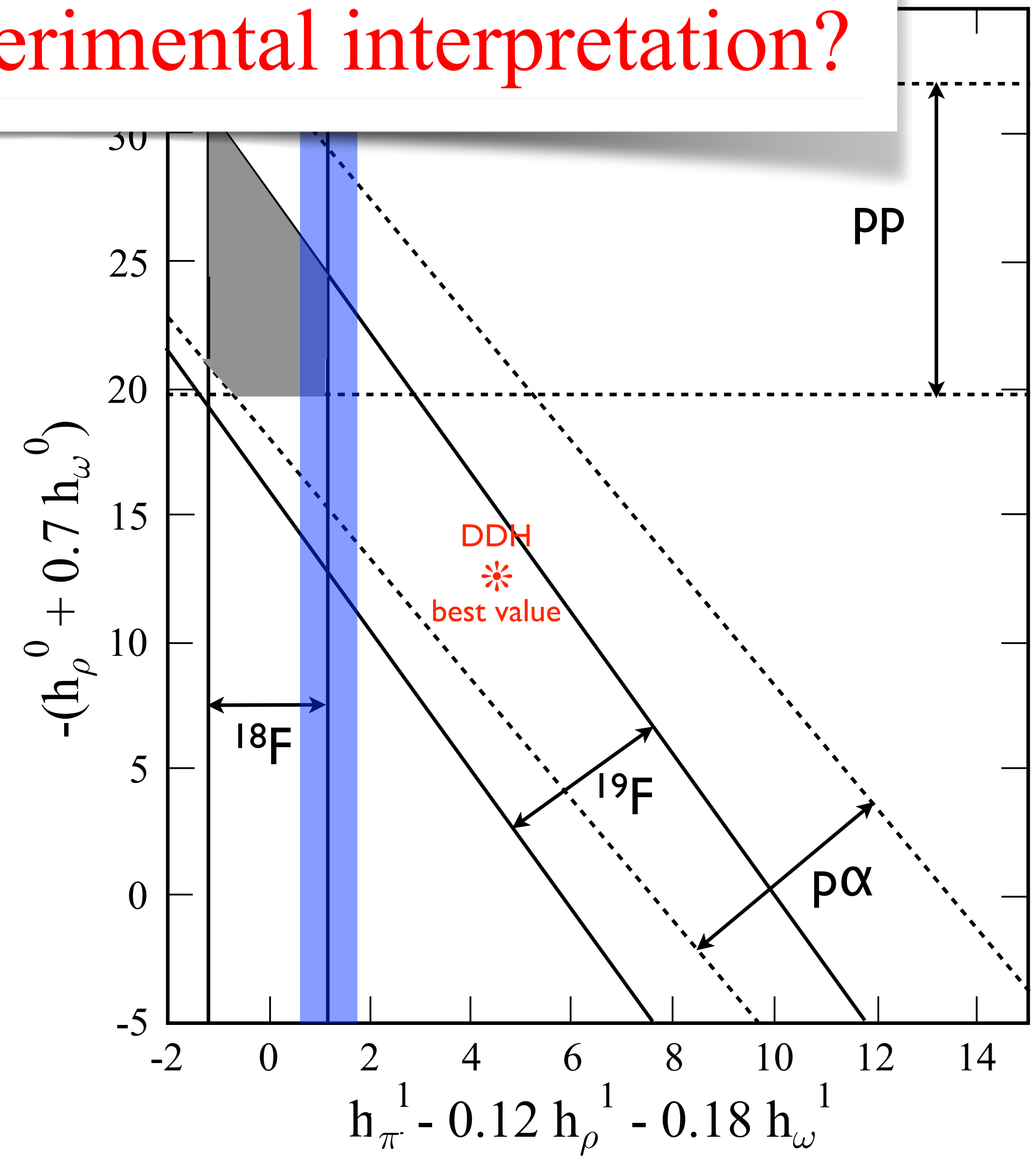
Haxton & Holstein
Prog. Part. Nucl. Phys., (2013)



(1) Anapole tensions

Difficulties of nuclear structure OR issues with APV experimental interpretation?





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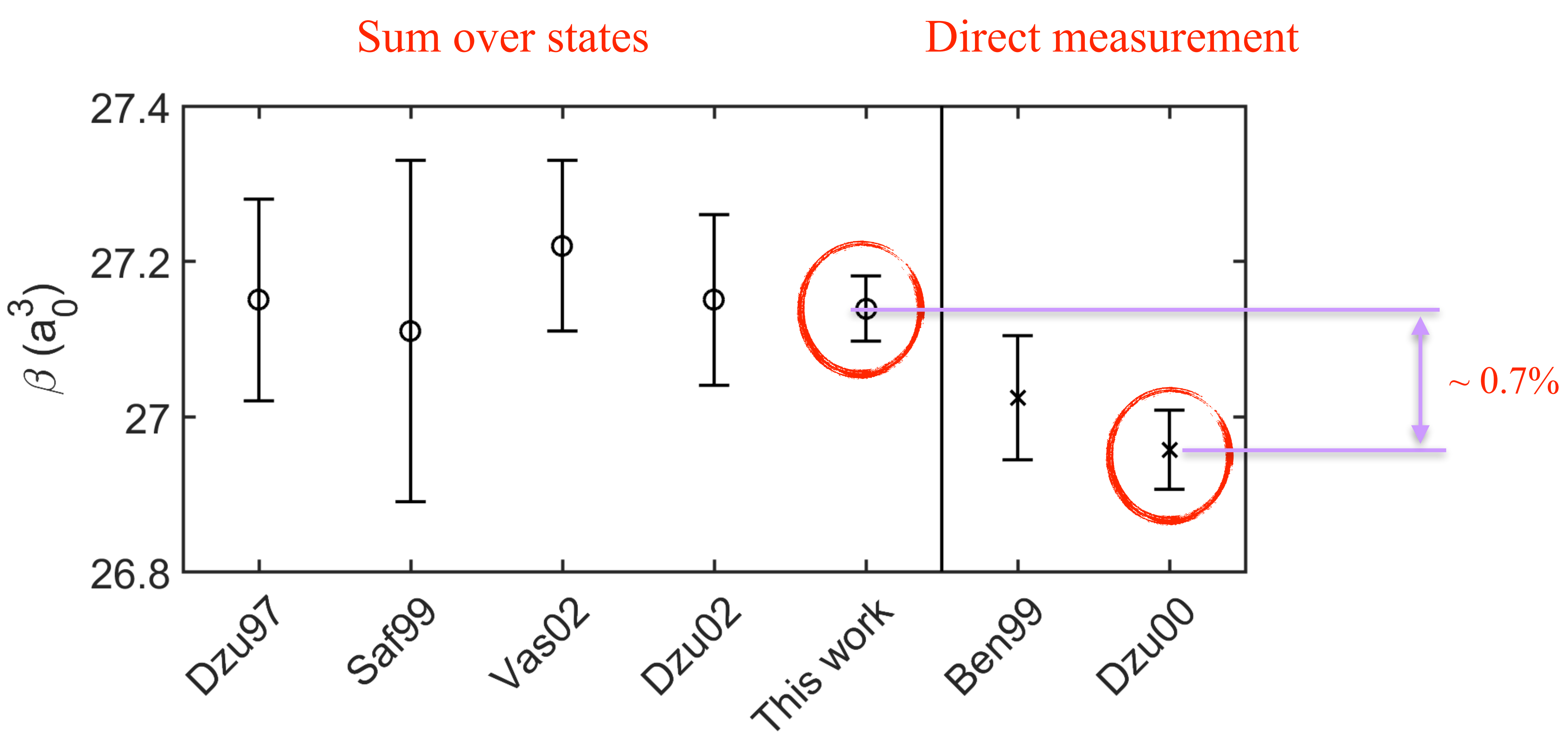
(2) Vector transition polarizability β

Measured: $$-\frac{\mathrm{Im}(E_{PV})}{\beta} = \begin{cases} 1.6349(80)\,\mathrm{mV/cm} & 6S_{F=4} \rightarrow 7S_{F=3} \\ 1.5576(77)\,\mathrm{mV/cm} & 6S_{F=3} \rightarrow 7S_{F=4} \end{cases}$$

Accurate (~0.1%) value of β is required to extract the PV amplitude



Toh… Elliot PRL 123, 073002 (2019)

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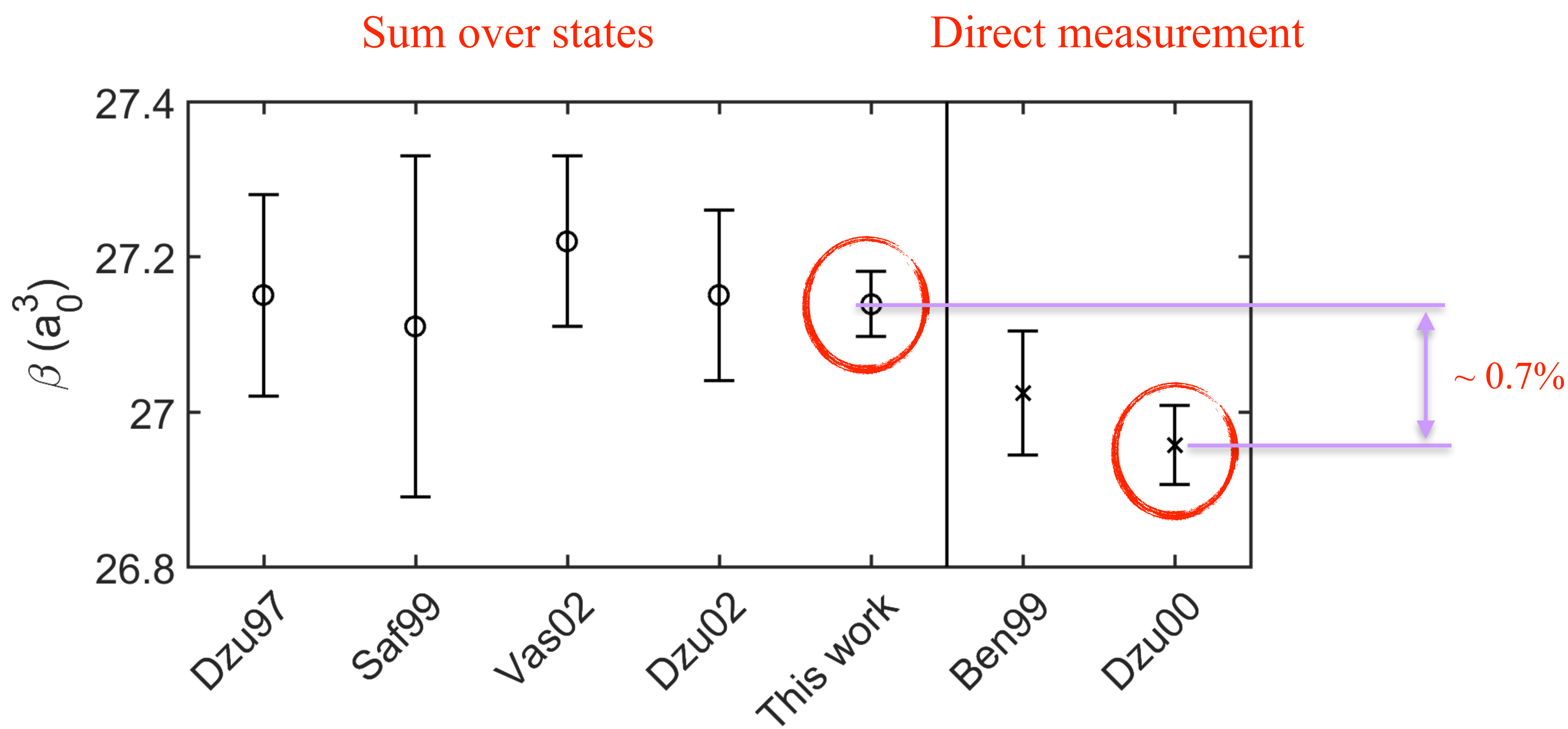

Why do the two approaches differ?

Hyperfine-induced corrections to transition polarizability

Static E-field + laser driving field $6S_{1/2} \rightarrow 7S_{1/2}$; experiment uses different F's

$$T_{i,f} = \langle f \,|\, (\mathbf{D}\cdot\mathbf{E}_s)\,\mathscr{R}\,(\mathbf{D}\cdot\mathbf{E}_L)\,|\, i\rangle + \mathrm{h\,.\,c\,.}$$

Re-coupling product of dipoles

New effect

$$T_{i,f} = \text{scalar} + \text{vector} + \text{tensor}$$

$$\propto \alpha \qquad \propto \beta \qquad \propto \gamma$$

Only due to hyperfine interaction

The effect turns out to be too small to explain the difference in beta and the anapole puzzle

D. Xiao, H. B. Tran Tan, and A. Derevianko, Phys. Rev. A 108, 032805 (2023)

(3) More accurate experimental results for dipole matrix elements [Purdue]

$$E_{\mathrm{PV}} = \sum_n \frac{\langle 7S_{1/2} | D | nP_{1/2} \rangle \langle nP_{1/2} | H_W | 6S_{1/2} \rangle}{E_{6S} - E_{nP_{1/2}}} + \mathrm{c.c.}(6S \leftrightarrow 7S)$$

H. B. Tran Tan and A. Derevianko, Phys. Rev. A 107, 042809 (2023)

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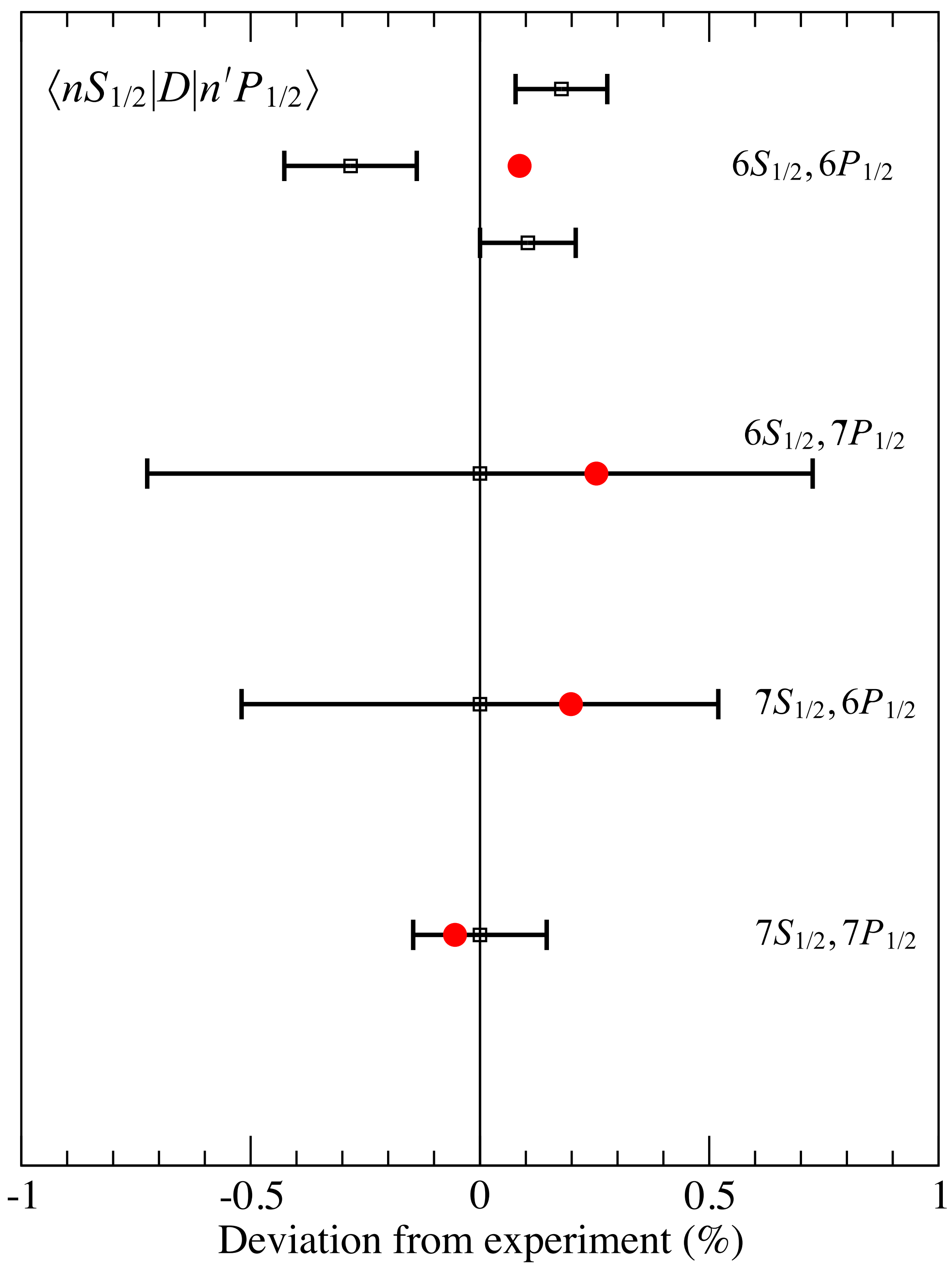

2010

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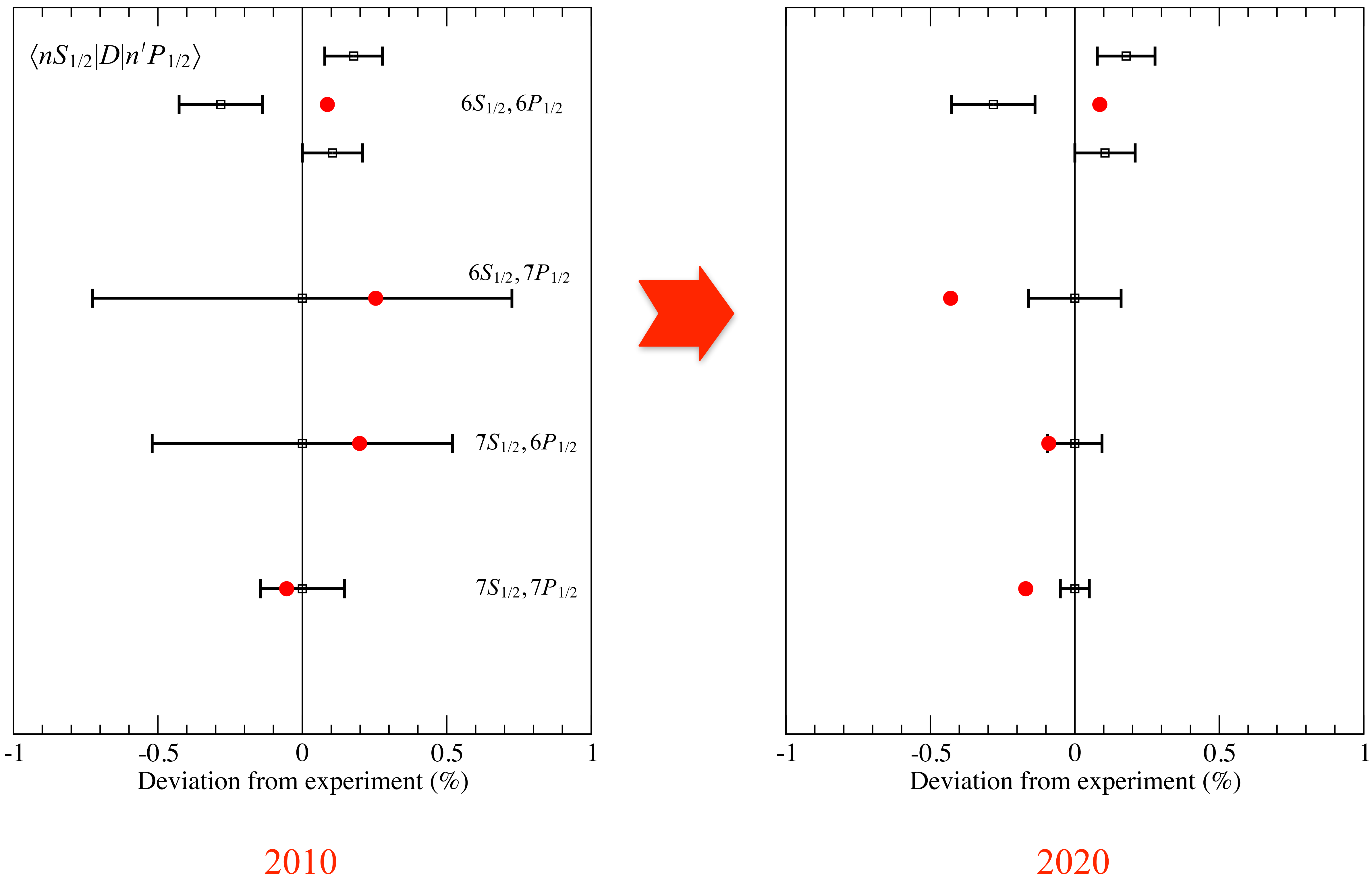
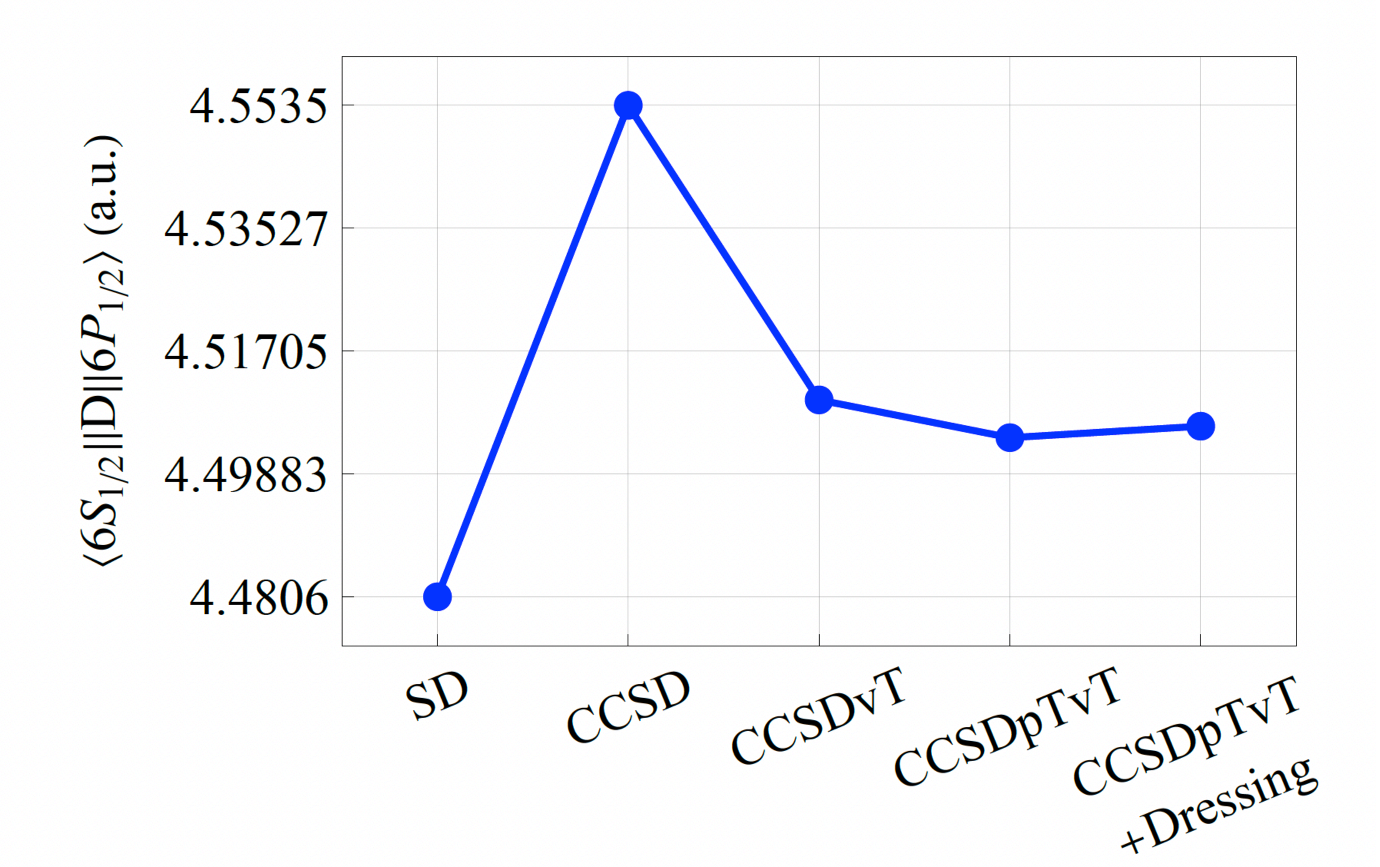


Toh… Elliot PRL 123, 073002 (2019)

More complete calculations of dipoles

- New, more powerful, 160-core 768Gb computational server (Templeton)
- Much larger basis sets, better control of numerical accuracy
- Systematic study of Cooper-like minima
- 28 matrix elements tabulated and accuracy is estimated
- Tension with experiments for several matrix elements



H. B. Tran Tan and A. Derevianko, Phys. Rev. A 107, 042809 (2023)

The victory lap

Quirk, Jacobsen, Damitz, Tanner, and Elliott PRL 132, 233201 (2024)

	$\langle 7s\|\|r\|\|7p_{1/2}\rangle$ (a_0^3)	$\langle 7s\|\|r\|\|7p_{3/2}\rangle$ (a_0^3)
This work	10.303 (3)	14.311 (3)
*Bennett *et al.* [14]	10.325 (5)	14.344 (7)
Reno — Tan *et al.* [13]	10.292 (6)	14.297 (10)
Roberts *et al.* [11, 12]	10.297 (23)	14.303 (33)
Safronova *et al.* [31]	10.310 (40)	14.323 (61)
Dzuba *et al.* [32]	10.285 (31)	14.286 (43)

TABLE III. Comparison of matrix elements $\langle 7s||r||7p_{1/2}\rangle$ and $\langle 7s||r||7p_{3/2}\rangle$. Experimental determinations are above the double line and theoretical are below. *These matrix elements were derived from the measurements of Bennett *et* al. [14] and reported in Ref. [9].

* Our values are 4-7 x more accurate than previous theories
* 5 sigma disagreement with Boulder expt value
* New Purdue experiment supports our value

(2') Vector transition polarizability β

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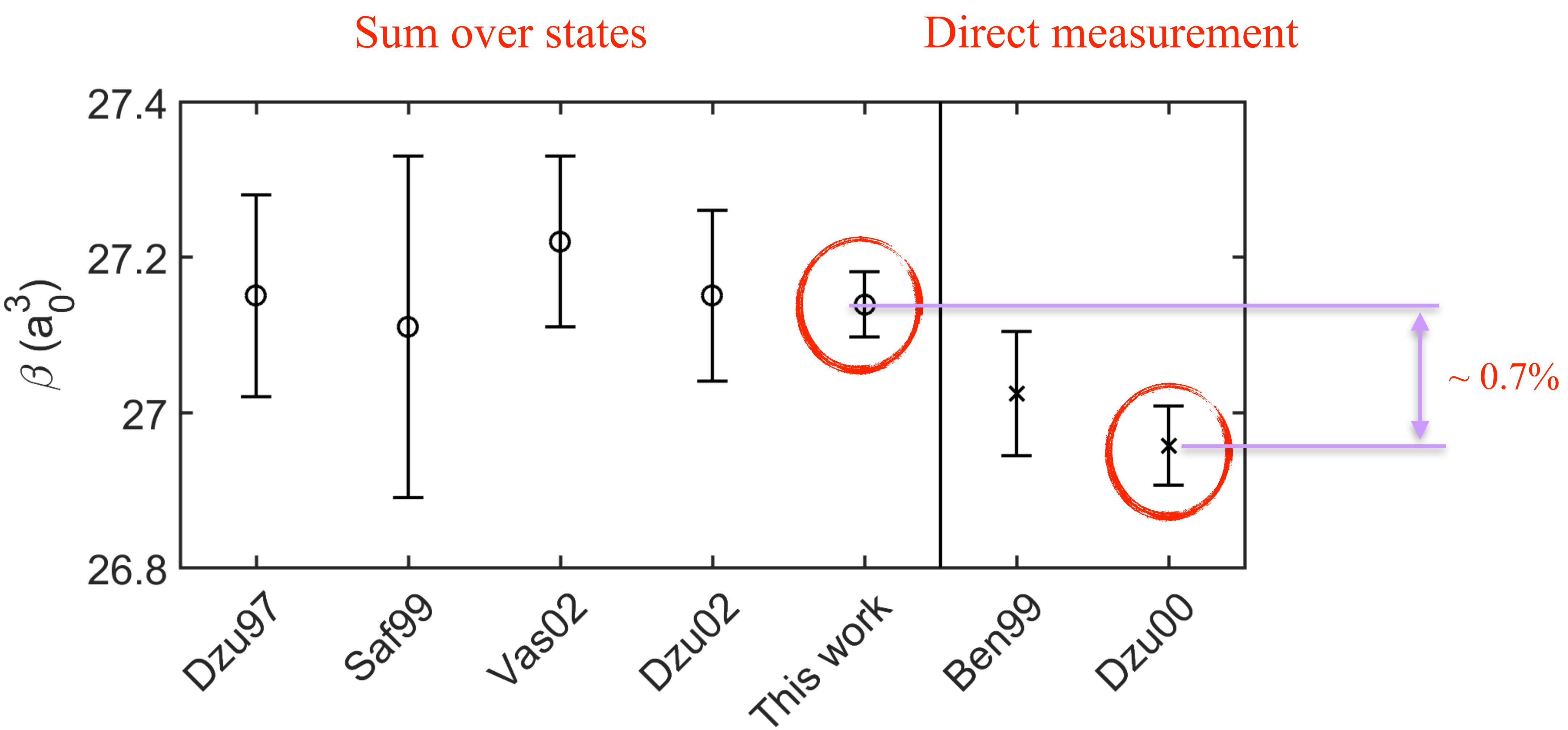
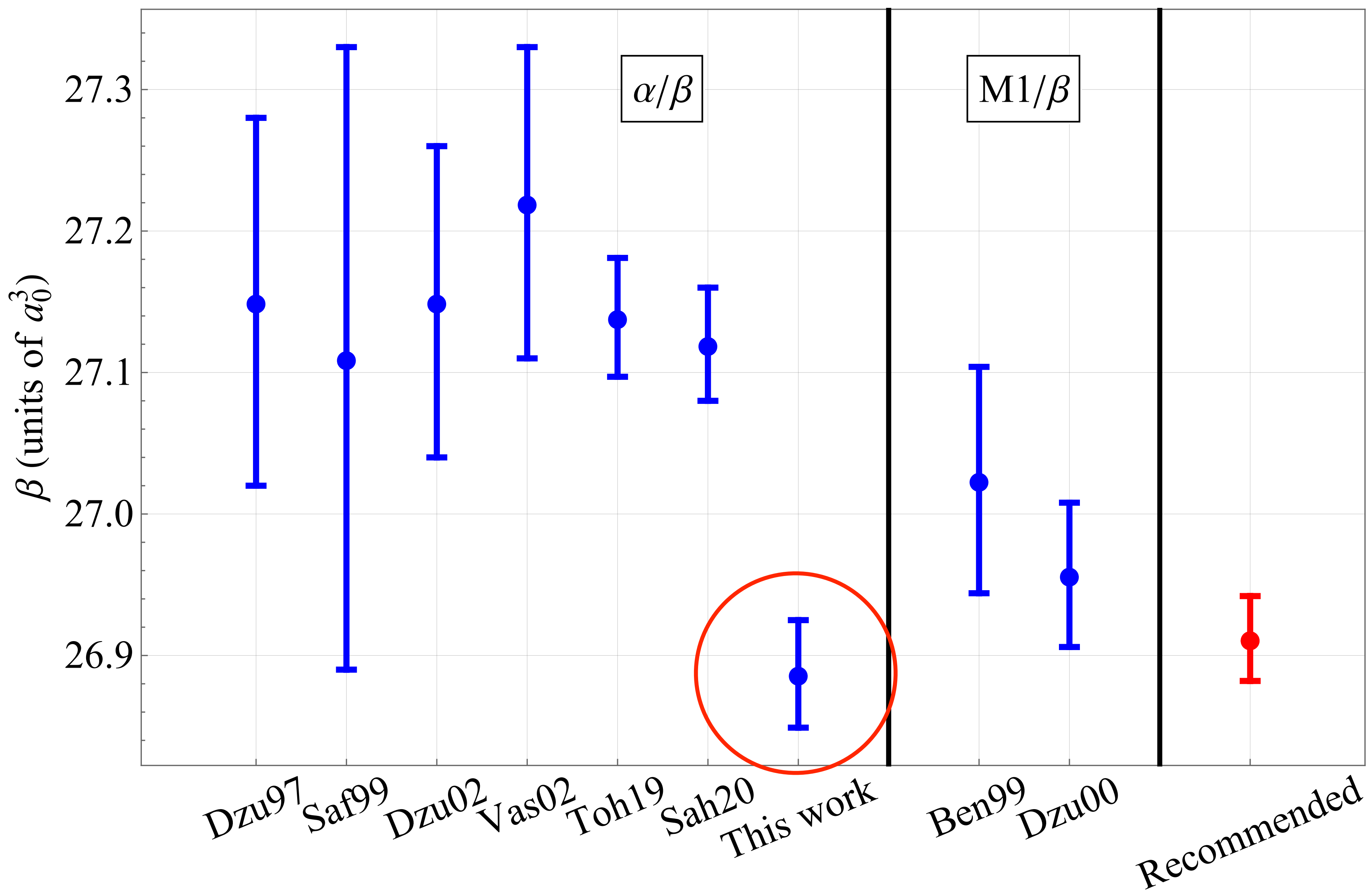


Toh… Elliot PRL 123, 073002 (2019)

Reconciliation of β



The tension between the two methods is resolved.
Reason: difference b/w theory and expt for the $\langle 6{,}7S_{1/2}|D|6{,}7P_{3/2}\rangle$ matrix elements
One of them was resolved in the theory favor by the Purdue experiment

H. B. Tran Tan, D. Xiao, and A. Derevianko PRA 108, 022808 (2023)

(5) New computational idea

$$E_{\rm PV} = \sum_n \frac{\langle 7S_{1/2}|D|nP_{1/2}\rangle\langle nP_{1/2}|H_W|6S_{1/2}\rangle}{E_{6S}-E_{nP_{1/2}}} + \text{c.c.}(6S \leftrightarrow 7S)$$

$$\text{Main}\,(n=6,7,8,9)[98\%] + \text{Tail}\,(n>9)[2\%]$$

Summation must be over the complete many-body basis: $\sum_n |nP_{1/2}\rangle\langle nP_{1/2}| = 1$

Approximation	Main	Tail
RPA	0.8705	0.0192
BO	0.8678	0.0242

=> Main and Tail must be computed in the same approximation

(5) How to reduce theory error further?

Table 1: Contributions to parity violating amplitude E_{PNC} for the $6S_{1/2} \to 7S_{1/2}$ transition in ^{133}Cs in units of $i|e|a_{\mathrm{B}}\left(-\frac{Q_W}{N}\right) \times 10^{-11}$.

Coulomb interaction	
Main ($n = 6 - 9$)	0.8823(18)
Tail	0.0175(18)
Total correlated	0.8998(25)
Corrections	
Breit, Ref. (*29*)	-0.0054(5)
QED, Ref. (*23*)	-0.0024(3)
Neutron skin, Ref. (*30*)	-0.0017(5)
$e - e$ weak interaction, Ref. (*11*)	0.0003
Final	0.8906(26)

Error bar is comparable to Main

(5) Parity-mixed CC approach

Use parity-mixed basis

$$\left(h_0 + V_{\mathrm{DHF}} + h_W\right)\phi_i = \varepsilon_i \phi_i$$

All single-particle orbitals include weak interaction

Feed into the CCSDvT code (remove parity selection rules)

All observables (dipoles, hyperfine constants, energies) will have the same accuracy as in the original CCSDvT code

Summation over intermediate states is gone!

$$E_{\mathrm{PV}} = \langle 7S_{1/2}(\mathrm{CCSDvT}-\mathrm{PM}) | D | 6S_{1/2}(\mathrm{CCSDvT}-\mathrm{PM}) \rangle$$

Price: increased computational complexity

With additional work, the goal is to attain 0.1% theoretical accuracy

Details of the formalism + low-order calculations in
H. B. Tran Tan, D. Xiao, and A. Derevianko, *Phys. Rev. A 105, 022803 (2022)*

Summary: Revisiting APV in Cs

(1) Tension for the ^{133}Cs anapole moment with the nuclear theory

(2) Tension for supporting quantities (vector transition polarizability) - **RESOLVED**

(3) More accurate dipole matrix elements

(4) New experimental efforts on measuring APV in Cs [Purdue]

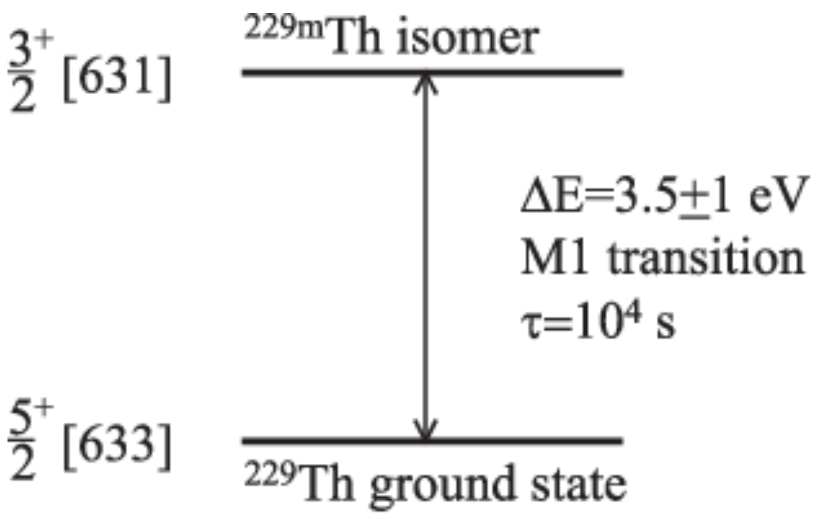
(5) New computational idea: parity-mixed CC (0.1% should be attainable)

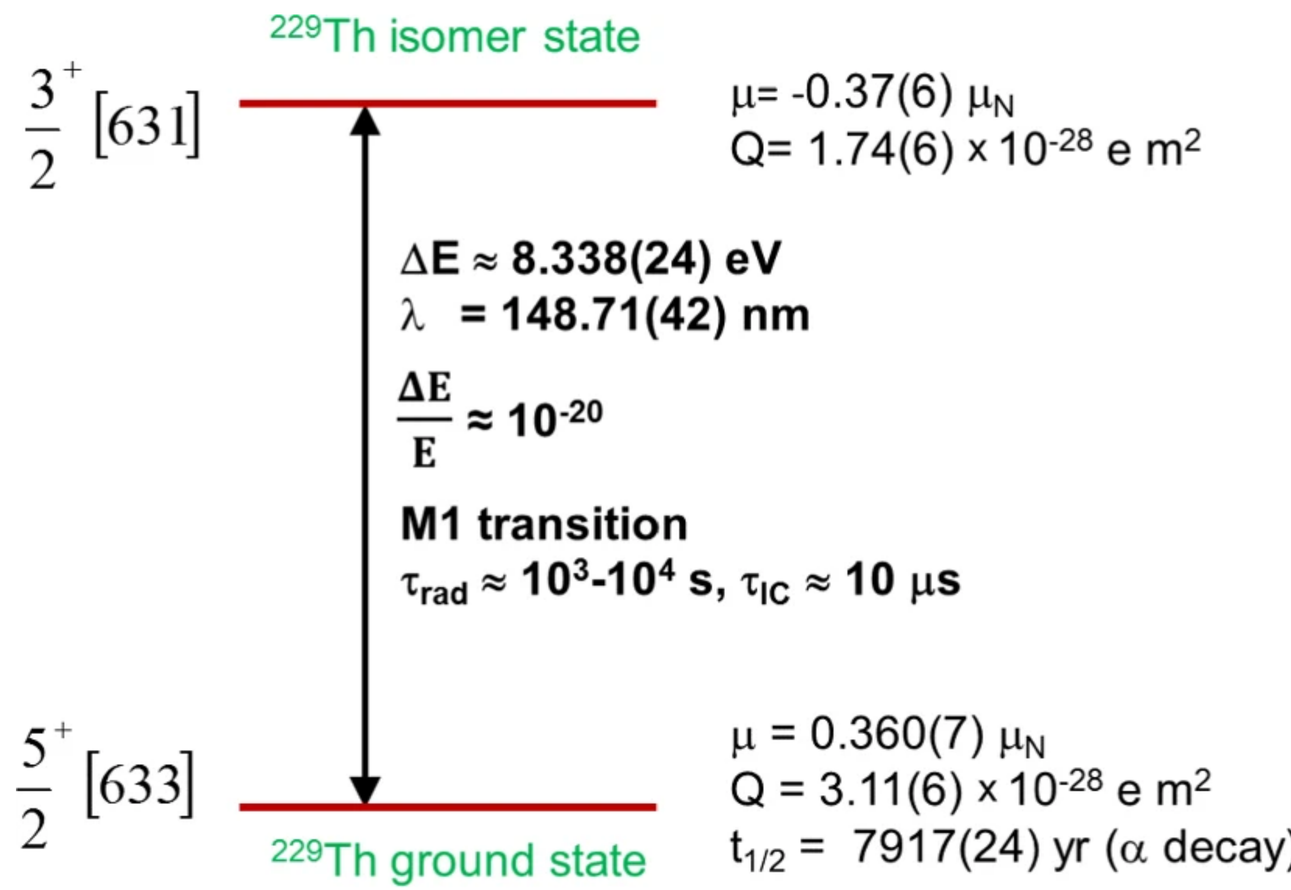
(6) New dark-sector motivations

Discussion

Tell me about nuclear clock (request at lunch)

Th-229 a.k.a. nuclear freak





Tkalya et al 1996
Peik&Tamm 2003

Single-Ion Nuclear Clock for Metrology at the 19th Decimal Place

C. J. Campbell, A. G. Radnaev, A. Kuzmich, V. A. Dzuba, V. V. Flambaum, and A. Derevianko

Phys. Rev. Lett. 108, 120802 (2012)

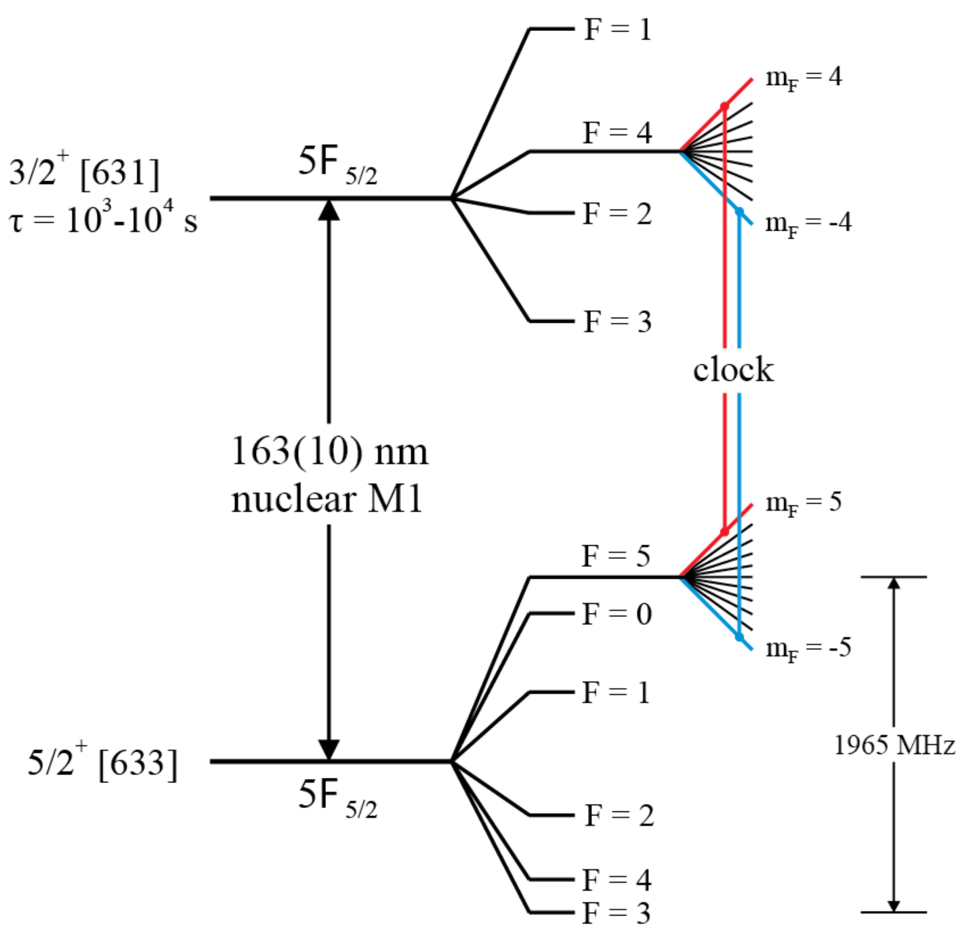


TABLE I. Estimated systematic error budget for a $^{229}Th^{3+}$ clock using realized single-ion clock technologies. Shifts and uncertainties are in fractional frequency units ($\Delta\nu/\nu_{clk}$) where $\nu_{clk} = 1.8$ PHz. See text for discussion.

Effect	|Shift| (10^{-20})	Uncertainty (10^{-20})
Excess micromotion	10	10
Gravitational	0	10
Cooling laser Stark	0	5
Electric quadrupole	3	3
Secular motion	5	1
Linear Doppler	0	1
Linear Zeeman	0	1
Background collisions	0	1
Blackbody radiation	0.013	0.013
Clock laser Stark	0	$\ll 0.01$
Trapping field Stark	0	$\ll 0.01$
Quadratic Zeeman	0	0
Total	18	15

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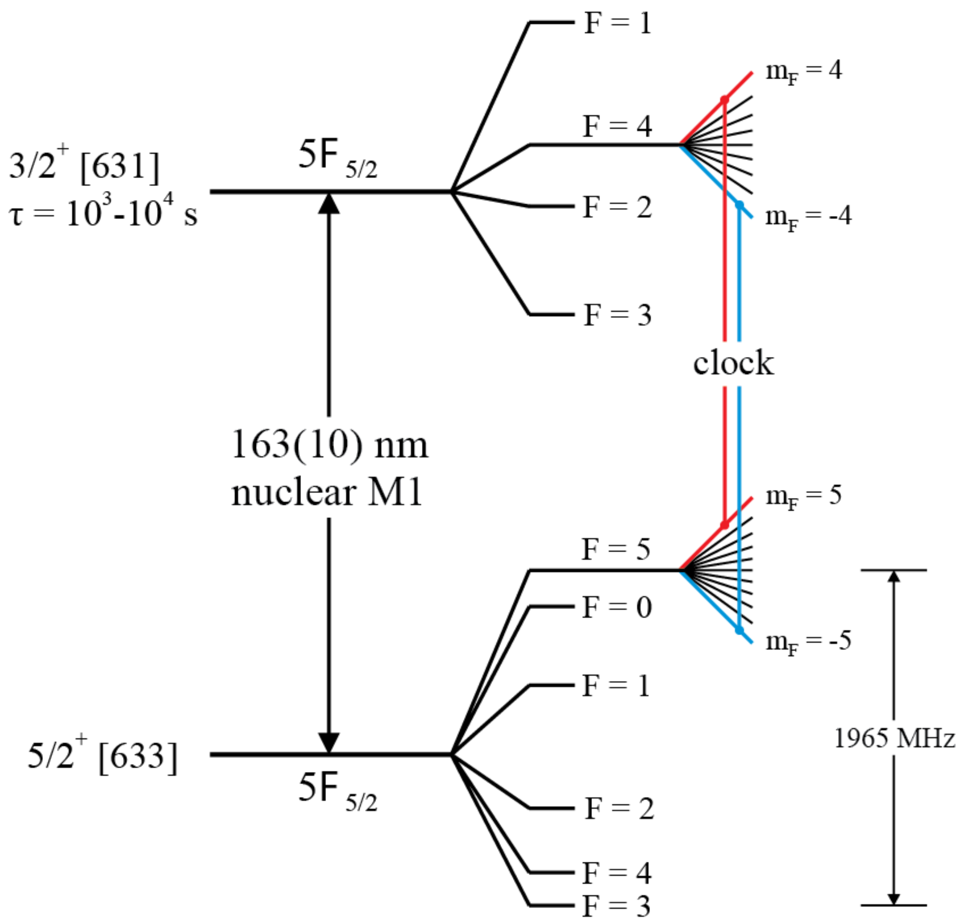

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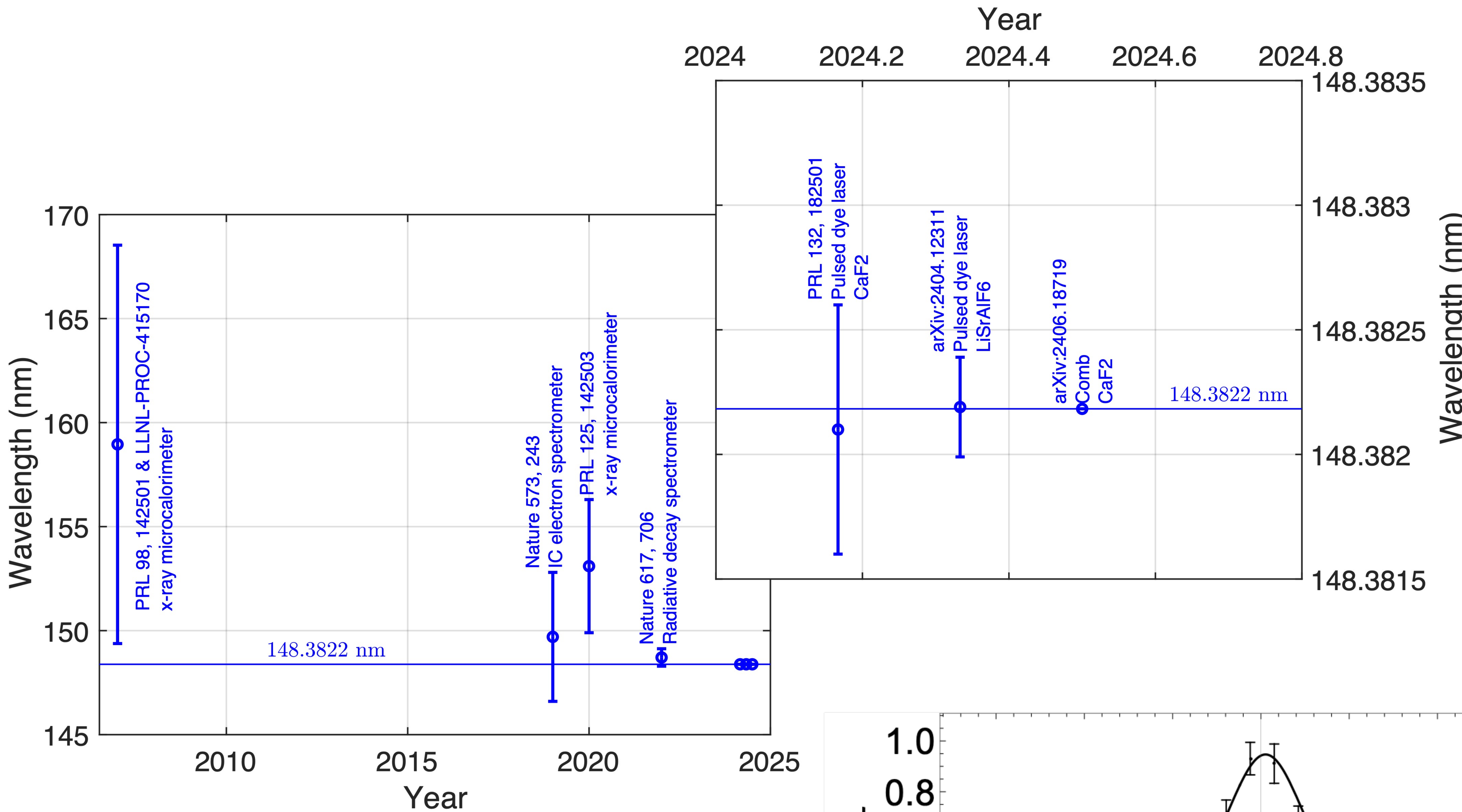
Total	18	15

Finally got it (20 years in the making)!



Now transition energy is measured to 12 sig. figs

Th-229 doped crystals