Tests of fundamental symmetries with atoms and molecules

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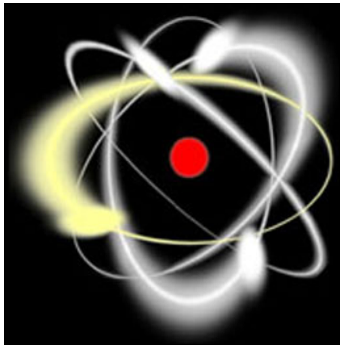
Listening to an atom



☐ Coulomb forces + Quantum Electro-Dynamics
=> a relatively simple interpretation

☐ Unprecedented control over internal and external degrees of freedom
precision 17-digit spectroscopy

Al^+ clock = several parts per quintillion (10^{18})

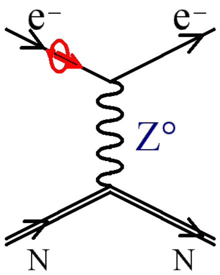
Precision AMO tests of fundamental symmetries

- Discrete:
  - Atomic parity violation (weak charge/anapole moments)
  - Electric dipole moments (T-odd, P-odd)
  - T-odd P-even interactions

- Continuous:
  - Lorentz
  - Time/space variation of fundamental constants (also Lorentz)

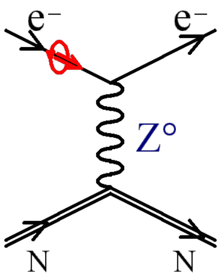
Other fundamental physics tests in AMO:
Equivalence principle, photon boson statistics, QED tests (alpha/e g-factor), Bell inequalities, …

Outline



Part I : Atomic Parity Violation

Part II: Nuclear clock and variation of fundamental constants



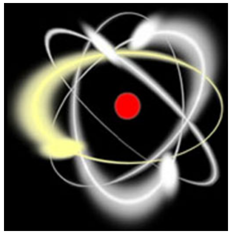
Part I

Atomic Parity Violation

Primer on evaluating theoretical error bars

Andrei Derevianko

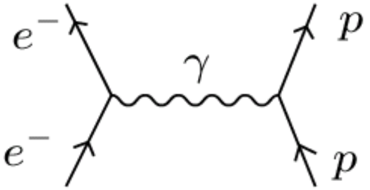
Atomic parity violation (APV)



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

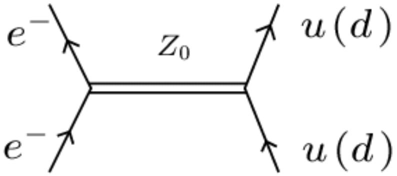
$[H_{\text{atomic}}, P]=0$ => Atomic stationary states are eigenstates of Parity

Electromagnetic



Conserve parity

Electroweak



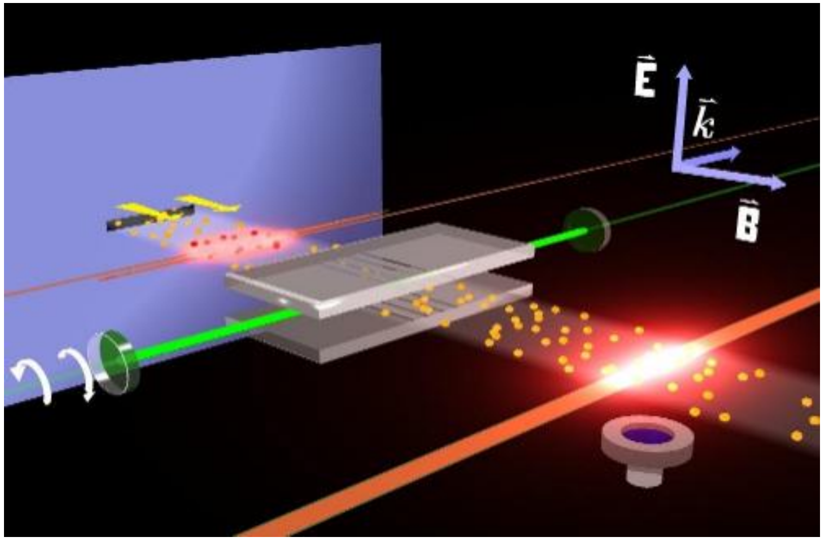
Do not conserve parity

Z-boson exchange spoils parity conservation

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

Atomic searches for new physics

Table top experiment with ^{133}Cs atoms
on parity violation
Boulder (C. Wieman group)

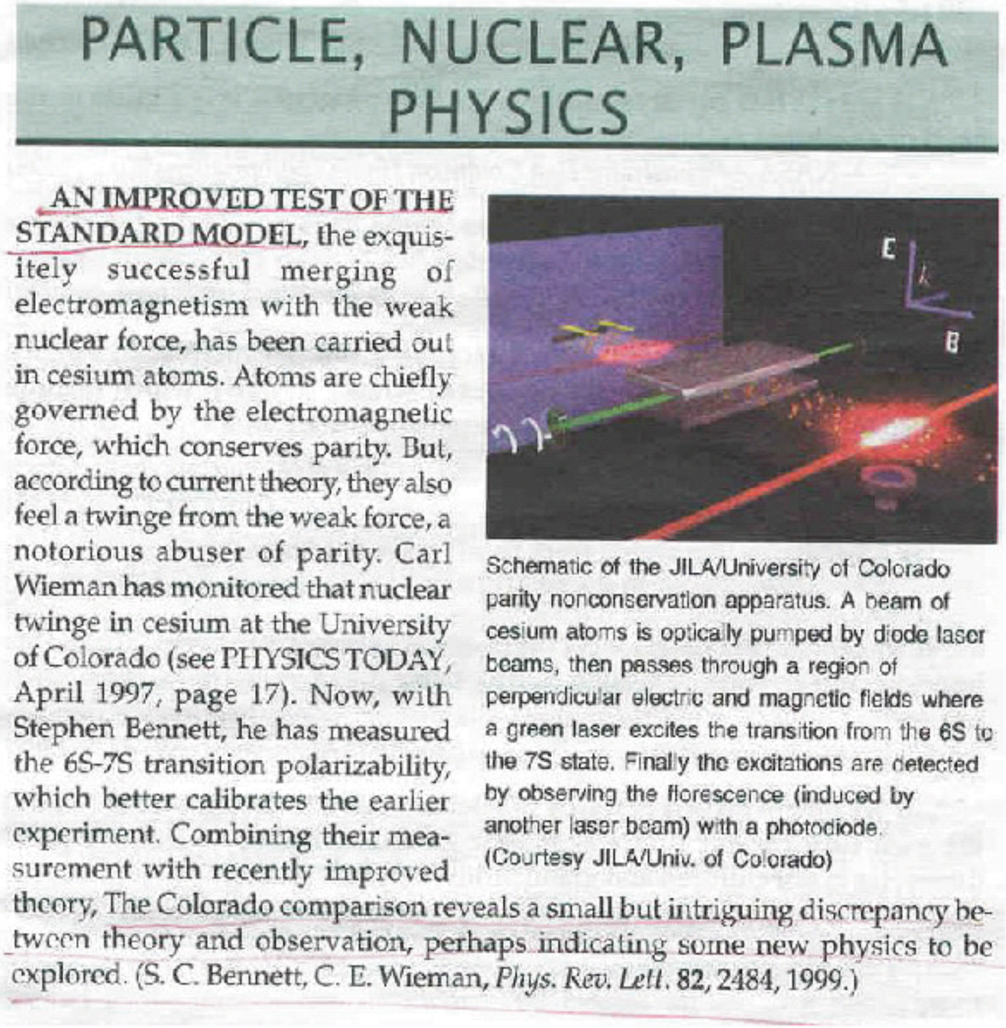


1 eV -> New physics constraints at 1 TeV mass scale

Atomic experiments are both unique and complementary to particle colliders

Cs PV experiment: Physics news (1999)

Annual survey of important physics stories



PARTICLE, NUCLEAR, PLASMA PHYSICS

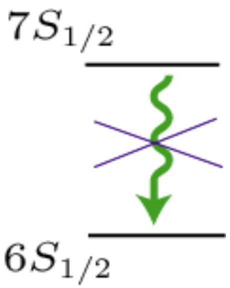
AN IMPROVED TEST OF THE STANDARD MODEL, the exquisitely successful merging of electromagnetism with the weak nuclear force, has been carried out in cesium atoms. Atoms are chiefly governed by the electromagnetic force, which conserves parity. But, according to current theory, they also feel a twinge from the weak force, a notorious abuser of parity. Carl Wieman has monitored that nuclear twinge in cesium at the University of Colorado (see PHYSICS TODAY, April 1997, page 17). Now, with Stephen Bennett, he has measured the 6S-7S transition polarizability, which better calibrates the earlier experiment. Combining their measurement with recently improved theory, The Colorado comparison reveals a small but intriguing discrepancy between theory and observation, perhaps indicating some new physics to be explored. (S. C. Bennett, C. E. Wieman, *Phys. Rev. Lett.* 82, 2484, 1999.)

Schematic of the JILA/University of Colorado parity nonconservation apparatus. A beam of cesium atoms is optically pumped by diode laser beams, then passes through a region of perpendicular electric and magnetic fields where a green laser excites the transition from the 6S to the 7S state. Finally the excitations are detected by observing the florescence (induced by another laser beam) with a photodiode. (Courtesy JILA/Univ. of Colorado)

"The Colorado comparison reveals a small but intriguing discrepancy between theory and observation, perhaps indicating some new physics to be explored"

Elementary particles community:
Numerous papers commenting on the discrepancy, e.g., extra Z-bosons

Parity-violating 7S-6S Amplitude in Cs



$$\langle 7S_{1/2}|D|6S_{1/2}\rangle \equiv 0$$

$$D=\sum_{i=1}^{N} -e\,\mathbf{r}_i$$

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

Weak interaction leads to an admixture of states of opposite parity (H_W is a pseudoscalar)

$$\overline{|6S_{1/2}\rangle} = |6S_{1/2}\rangle + \sum_m |mP_{1/2}\rangle \frac{\langle mP_{1/2}|H_W|6S_{1/2}\rangle}{E_{6S}-E_{mP_{1/2}}}$$

Similarly for $\overline{|7S_{1/2}\rangle}$

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

$$\sum_m \frac{\langle 7S_{1/2}|D|mP_{1/2}\rangle\langle mP_{1/2}|H_W|6S_{1/2}\rangle}{E_{6S}-E_{mP_{1/2}}} + \text{c.c.}(6S \leftrightarrow 7S)$$

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

Weak charge extraction

Electron-quark PV interaction (exchange of virtual Z^0 boson)

$$H_W = \frac{G_F}{\sqrt{2}}\left(\bar{e}\gamma_\mu\gamma_5 e\right)\left\{C_{1u}\bar{u}\gamma^\mu u + C_{1d}\bar{d}\gamma^\mu d\right\} + \ldots$$

In electronic sector

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

Weak charge

neutron distribution

PV signal

$$E_{PV} = k_{PV}\,Q_W^{\mathrm{inferred}}$$

measured

atomic-structure calculations

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

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

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

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

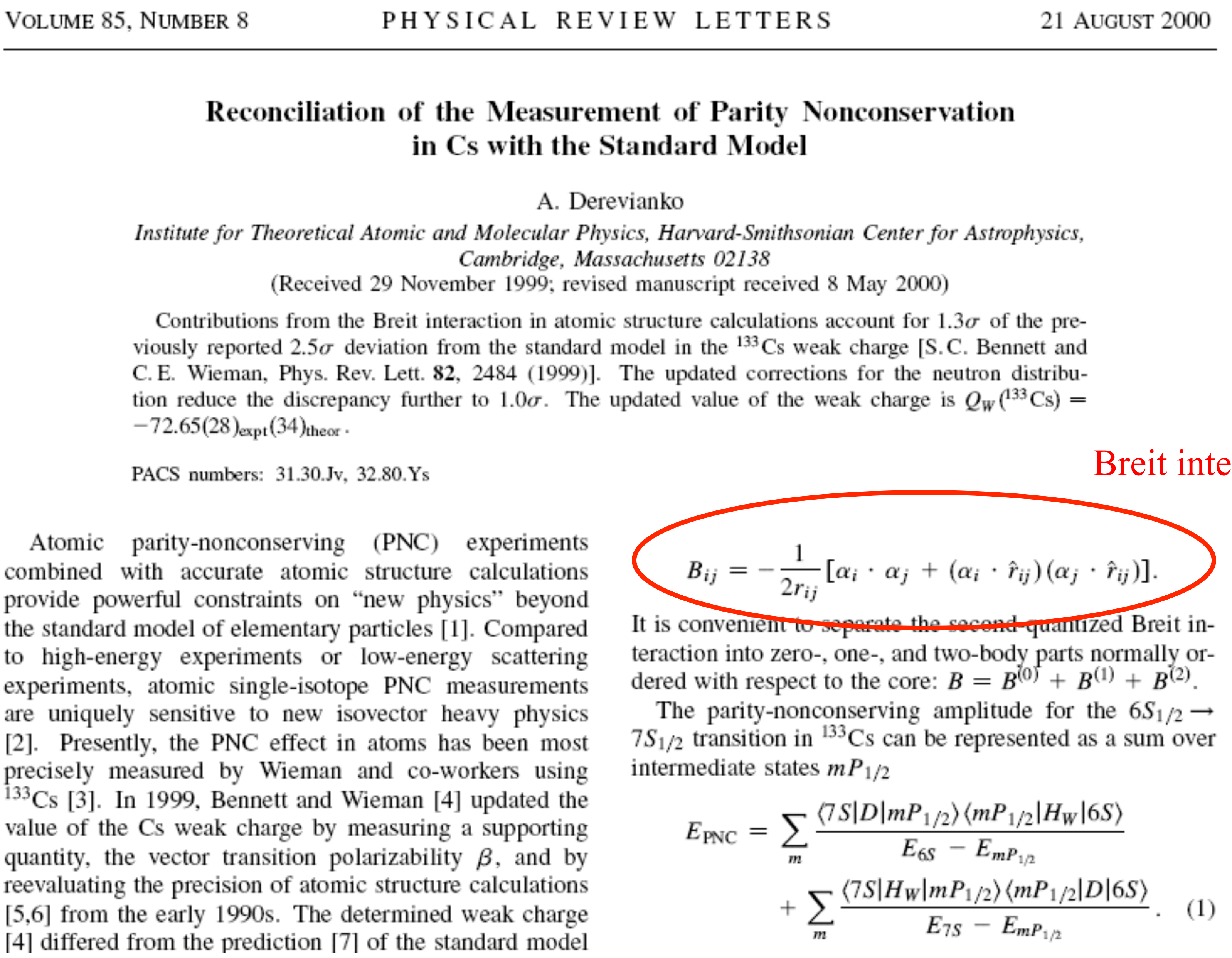
$$Q_W^{\mathrm{inferred}} \neq Q_W^{\mathrm{SM}}$$

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)



VOLUME 85, NUMBER 8 PHYSICAL REVIEW LETTERS 21 AUGUST 2000

Reconciliation of the Measurement of Parity Nonconservation in Cs with the Standard Model

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(Received 29 November 1999; revised manuscript received 8 May 2000)

Contributions from the Breit interaction in atomic structure calculations account for 1.3σ of the previously reported 2.5σ deviation from the standard model in the ^{133}Cs weak charge [S. C. Bennett and C. E. Wieman, Phys. Rev. Lett. **82**, 2484 (1999)]. The updated corrections for the neutron distribution reduce the discrepancy further to 1.0σ. The updated value of the weak charge is $Q_W(^{133}\mathrm{Cs}) = -72.65(28)_{\mathrm{expt}}(34)_{\mathrm{theor}}$.

PACS numbers: 31.30.Jv, 32.80.Ys

Atomic parity-nonconserving (PNC) experiments combined with accurate atomic structure calculations provide powerful constraints on "new physics" beyond the standard model of elementary particles [1]. Compared to high-energy experiments or low-energy scattering experiments, atomic single-isotope PNC measurements are uniquely sensitive to new isovector heavy physics [2]. Presently, the PNC effect in atoms has been most precisely measured by Wieman and co-workers using ^{133}Cs [3]. In 1999, Bennett and Wieman [4] updated the value of the Cs weak charge by measuring a supporting quantity, the vector transition polarizability β, and by reevaluating the precision of atomic structure calculations [5,6] from the early 1990s. The determined weak charge [4] differed from the prediction [7] of the standard model

Breit interaction

$$B_{ij} = -\frac{1}{2r_{ij}}[\alpha_i \cdot \alpha_j + (\alpha_i \cdot \hat{r}_{ij})(\alpha_j \cdot \hat{r}_{ij})].$$

It is convenient to separate the second-quantized Breit interaction into zero-, one-, and two-body parts normally ordered with respect to the core: $B = B^{(0)} + B^{(1)} + B^{(2)}$.

The parity-nonconserving amplitude for the $6S_{1/2} \rightarrow 7S_{1/2}$ transition in ^{133}Cs can be represented as a sum over intermediate states $mP_{1/2}$

$$E_{\mathrm{PNC}} = \sum_m \frac{\langle 7S|D|mP_{1/2}\rangle\langle mP_{1/2}|H_W|6S\rangle}{E_{6S} - E_{mP_{1/2}}} + \sum_m \frac{\langle 7S|H_W|mP_{1/2}\rangle\langle mP_{1/2}|D|6S\rangle}{E_{7S} - E_{mP_{1/2}}}. \quad (1)$$

Deviation from the Standard Model in PV with ^{133}Cs (2005)

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

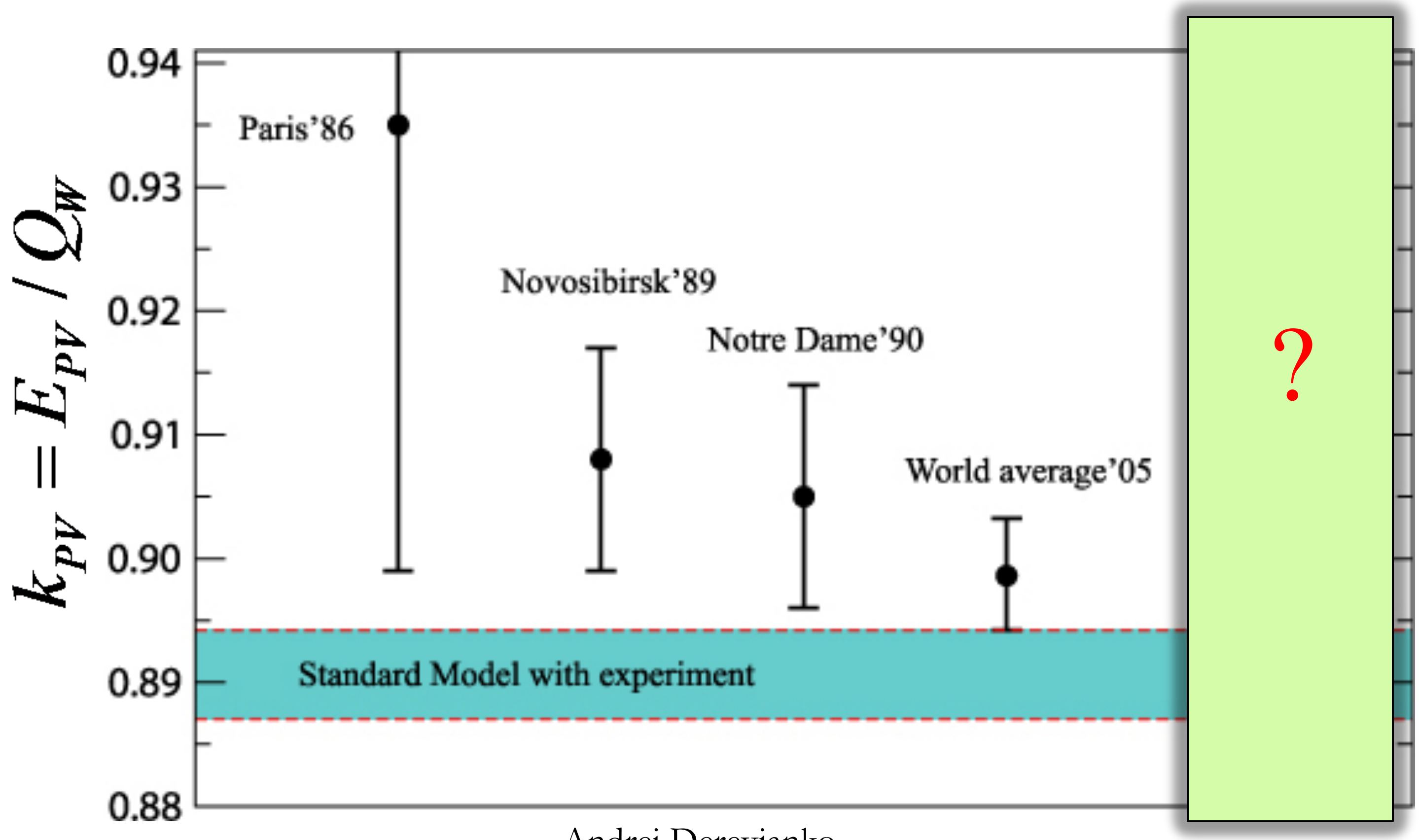
1999 Based on decade-old calculations by Dzuba *et al.* and Blundell *et al.*	2.5σ	Bennett & Wieman 1999
Breit interaction	-1.2σ	Derevianko (2000) , Dzuba *et al* (2001), Kozlov *et al* (2001); Shabaev *et al.* (2005)
Vacuum polarization (+ 0.8 σ) Vertex/self-energy (-1.3 σ)	-0.5σ	Johnson *et al.* (2002);Milstein & 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->0, virtual exc. of the giant nuc. res.	-0.08 σ	Sushkov & Flambaum (1978) Milstein,Sushkov&Terekhov (2002)
Total deviation	1.0 σ	

Theoretical progress

$$E_{PV} = k_{PV}\, Q_W^{\text{inferred}}$$

measured

atomic-structure calculations



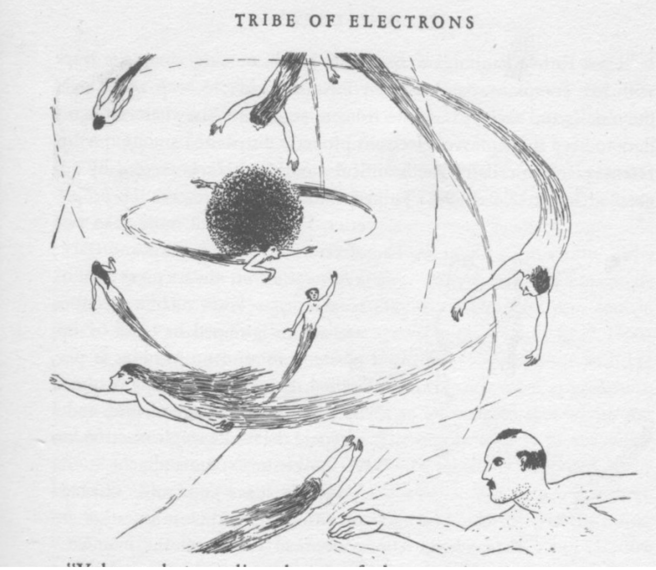
$$\sigma_Q = \sqrt{\left(\sigma_{\text{expt}}\right)^2 + \left(\sigma_{\text{theor}}\right)^2}$$

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

How to reduce σ?

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

Why is it so difficult?



Cs atom: correlated motion of 55 electrons
55x3=165 coordinates
For a coarse 10-point grid per dimension

# of points in Hilbert space 10^{165}

Exceeds estimated number of atoms in the Universe

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

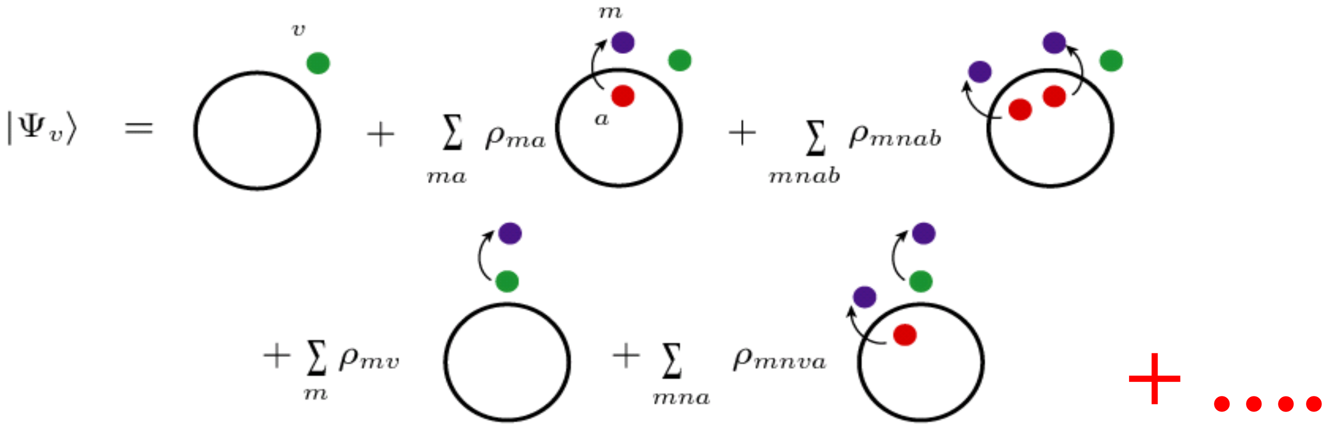
Many-body perturbation theory

Treat interaction beyond the Hartree-Fock as a perturbation

Technically difficult task: 100 Gb of storage, several weeks of CPU time

Coupled cluster method as a systematic approach

The accuracy of calculations based on SD method for PNC amplitude in Cs is ~ 1% (Blundell, Johnson, Sapirstein 1990)



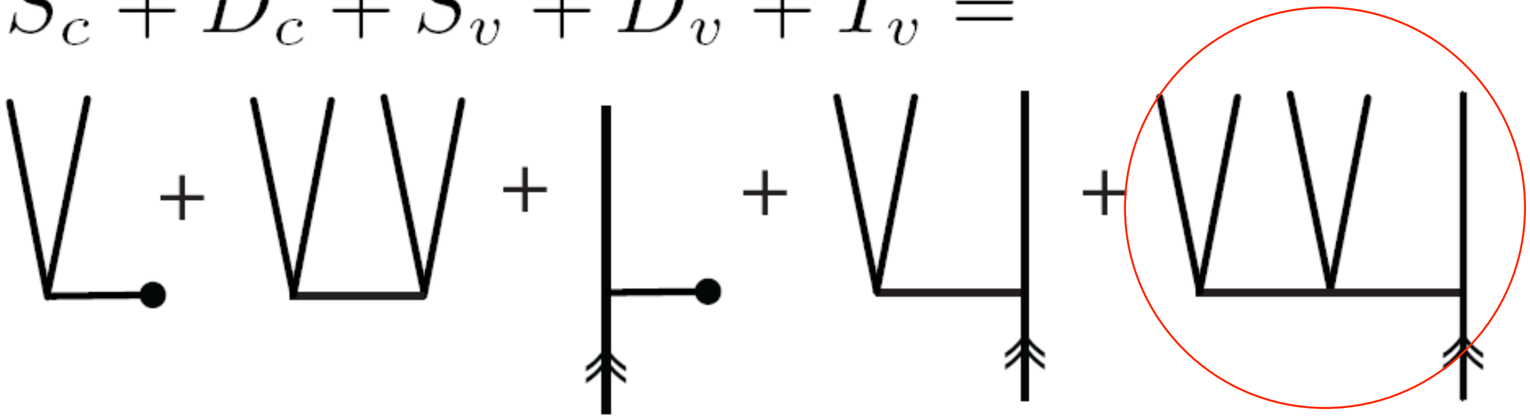
$$H|\Psi_v\rangle = E|\Psi_v\rangle$$

Triple and higher-rank excitations are missing from the exact wavefunction. =>

Next systematic step: include triples + non-linear product states.

Our CCSDvT approximation

$$K \equiv S_c + D_c + S_v + D_v + T_v =$$



$$\left|\Psi_v\right\rangle = \left(1 + K + \frac{1}{2!} N\left[K^2\right] + \ldots\right)\left|\Psi_v^{(0)}\right\rangle$$

⇨ 1,000-fold increase in computational complexity over previous calculations (ND:100 Mb → 100 Gb)

Our method

- *Ab initio* relativistic many-body method
- Based on coupled-cluster scheme (additional inclusion of triple excitations + non-linear terms)
- 1,000-fold increase in computational complexity over previous calculations (100 Mb → 100 Gb)
- Code quality control: 2 person team + symbolic tools
- Exact for 3e lithium: 0.01% accuracy demonstrated

Eight years, dozen of papers, 3,648 diagrams later …

PV amplitude

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

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

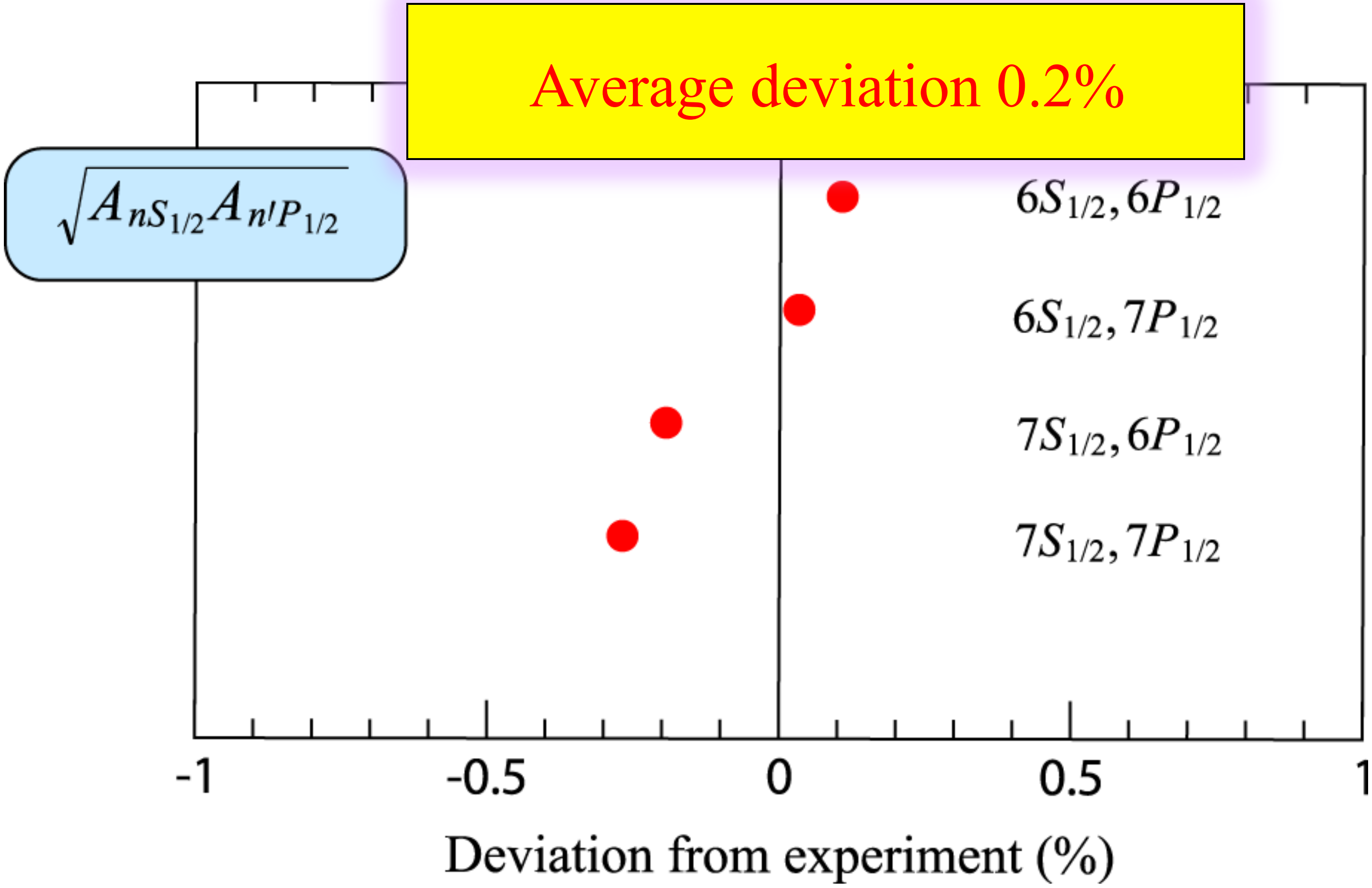
Accuracy is important

Main +tail

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

99% of the sum comes from n=6,7,8,9 (main term CCSDvT)

Theoretical accuracy: weak interaction

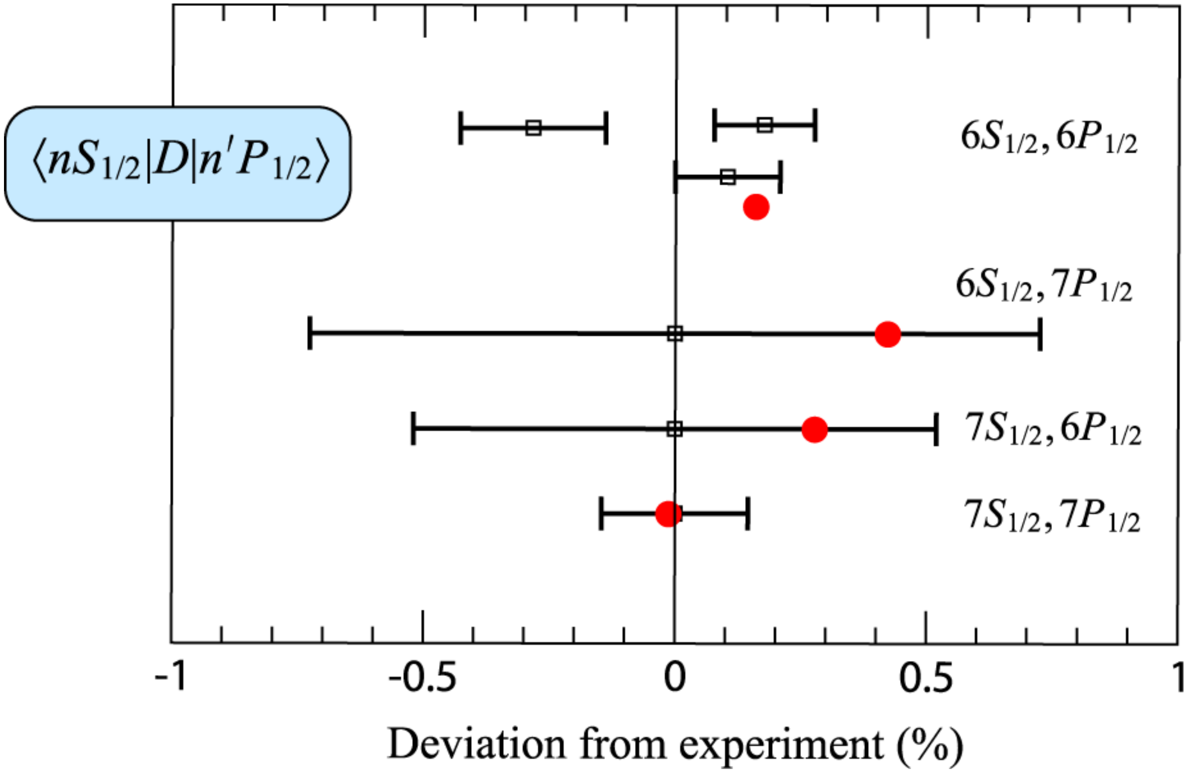


Average deviation 0.2%

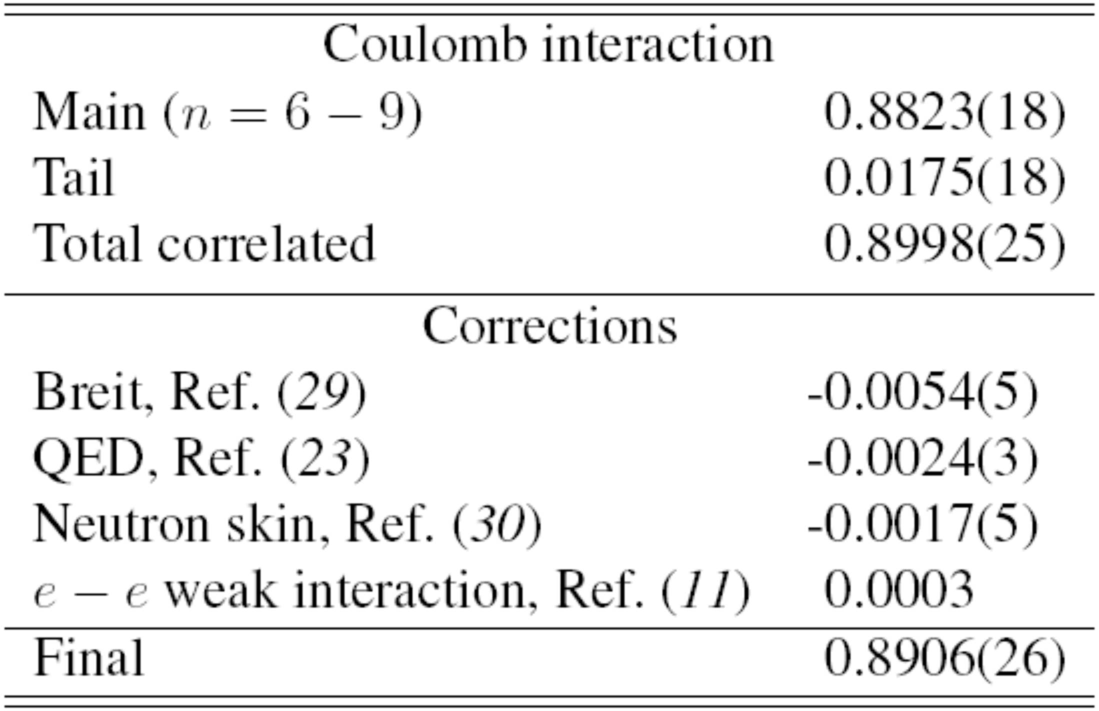
$\sqrt{A_{nS_{1/2}}A_{n'P_{1/2}}}$

Theoretical accuracy: dipoles

$\langle nS_{1/2}|D|n'P_{1/2}\rangle$

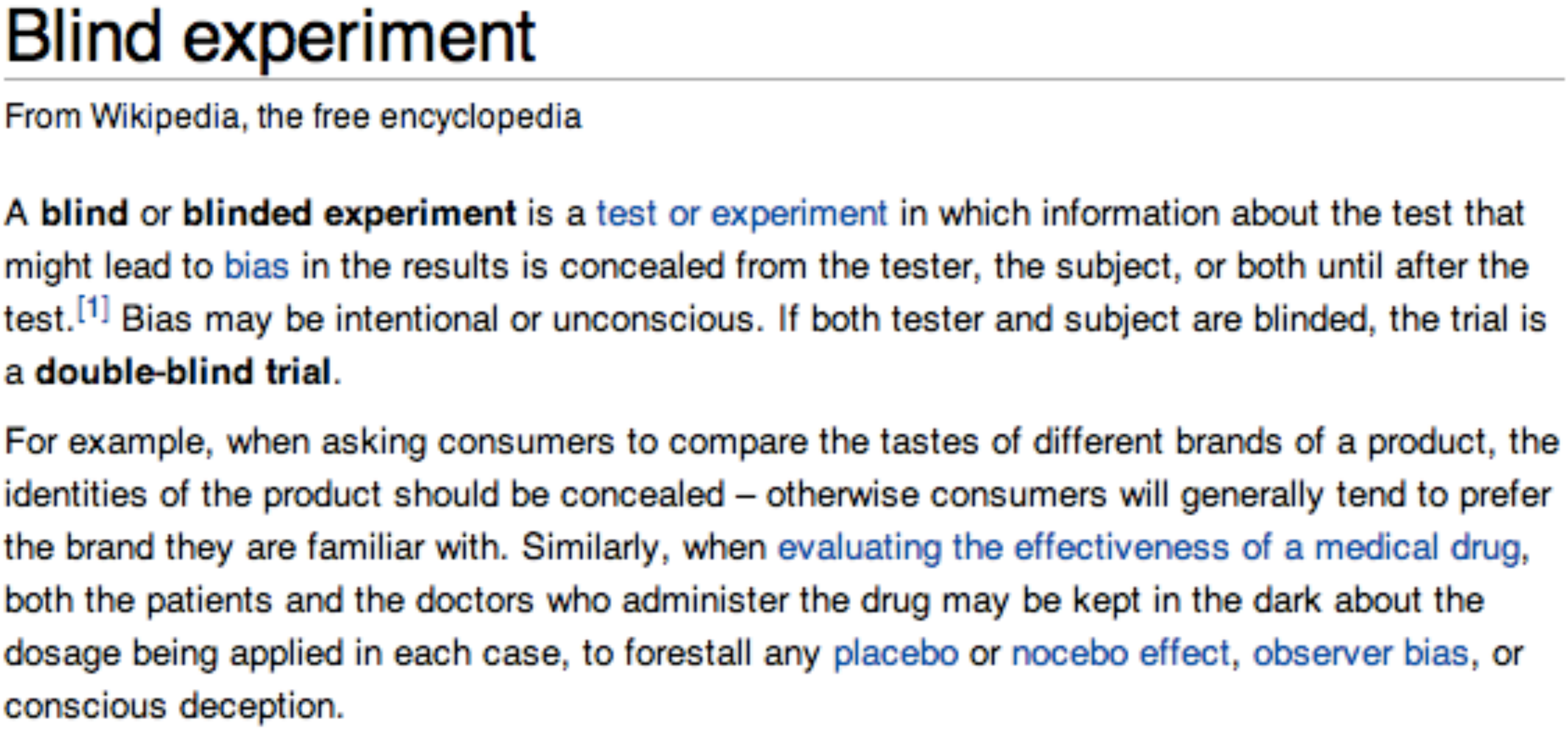


PV Amplitude



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)

Overall error 0.27% - better than the experiment



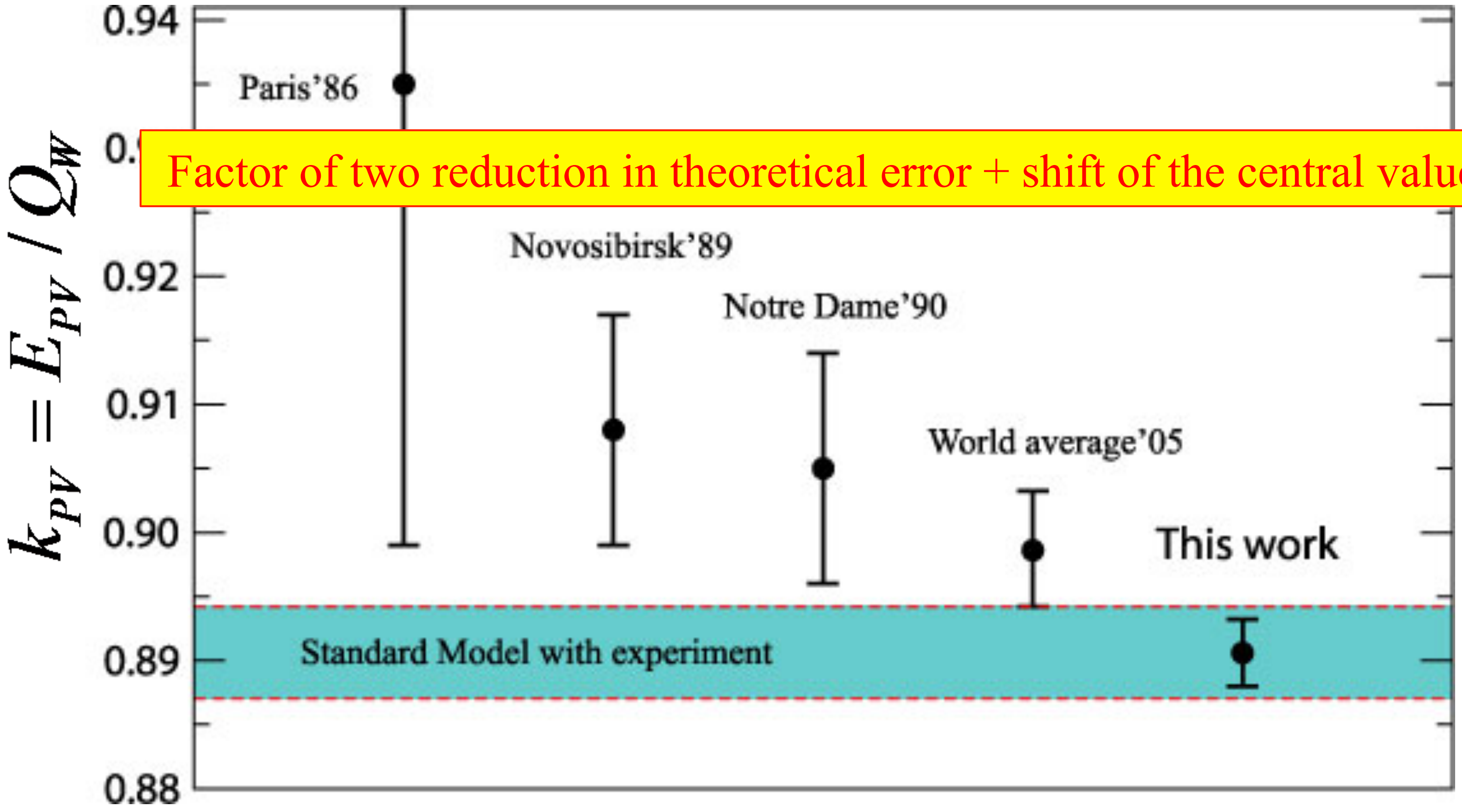
Blind experiment

From Wikipedia, the free encyclopedia

A **blind** or **blinded experiment** is a test or experiment in which information about the test that might lead to bias in the results is concealed from the tester, the subject, or both until after the test.[1] Bias may be intentional or unconscious. If both tester and subject are blinded, the trial is a **double-blind trial**.

For example, when asking consumers to compare the tastes of different brands of a product, the identities of the product should be concealed – otherwise consumers will generally tend to prefer the brand they are familiar with. Similarly, when evaluating the effectiveness of a medical drug, both the patients and the doctors who administer the drug may be kept in the dark about the dosage being applied in each case, to forestall any placebo or nocebo effect, observer bias, or conscious deception.

Theoretical progress

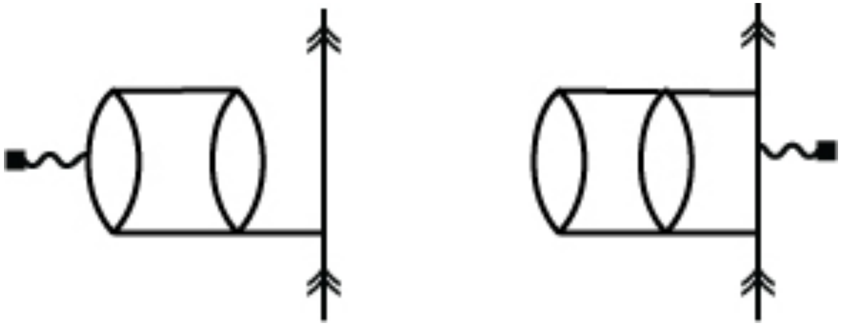


Factor of two reduction in theoretical error + shift of the central value

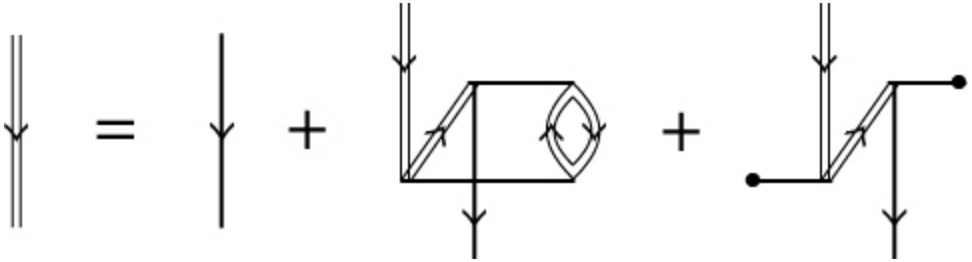
S. G. Porsev, K. Beloy and A. Derevianko, *Phys. Rev. Lett. 102, 181601 (2009)*
S. G. Porsev, K. Beloy and A. Derevianko, *Phys. Rev. D 82, 036008 (2010)*

Reasons for the shift of E_{PV}

(a) Direct contribution of triples to matrix elements (0.3%)

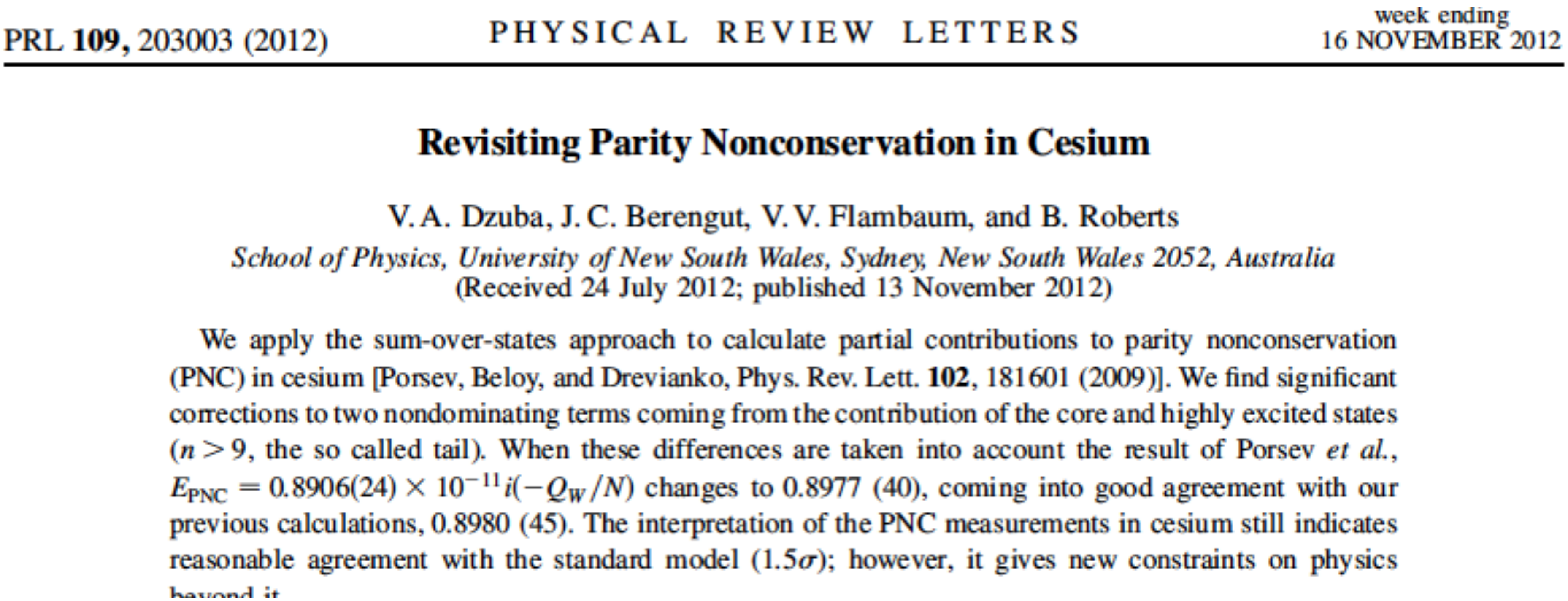


(b) line-dressing of matrix elements (0.3%)



(c) Consistent removal of Breit and QED effects from experimental energies (0.3%)

New twist in the Cs saga (2012)



PRL **109,** 203003 (2012) PHYSICAL REVIEW LETTERS week ending 16 NOVEMBER 2012

Revisiting Parity Nonconservation in Cesium

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(Received 24 July 2012; published 13 November 2012)

We apply the sum-over-states approach to calculate partial contributions to parity nonconservation (PNC) in cesium [Porsev, Beloy, and Derevianko, Phys. Rev. Lett. **102**, 181601 (2009)]. We find significant corrections to two nondominating terms coming from the contribution of the core and highly excited states ($n > 9$, the so called tail). When these differences are taken into account the result of Porsev *et al.*, $E_{\mathrm{PNC}} = 0.8906(24) \times 10^{-11} i(-Q_W/N)$ changes to 0.8977 (40), coming into good agreement with our previous calculations, 0.8980 (45). The interpretation of the PNC measurements in cesium still indicates reasonable agreement with the standard model (1.5σ); however, it gives new constraints on physics beyond it

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

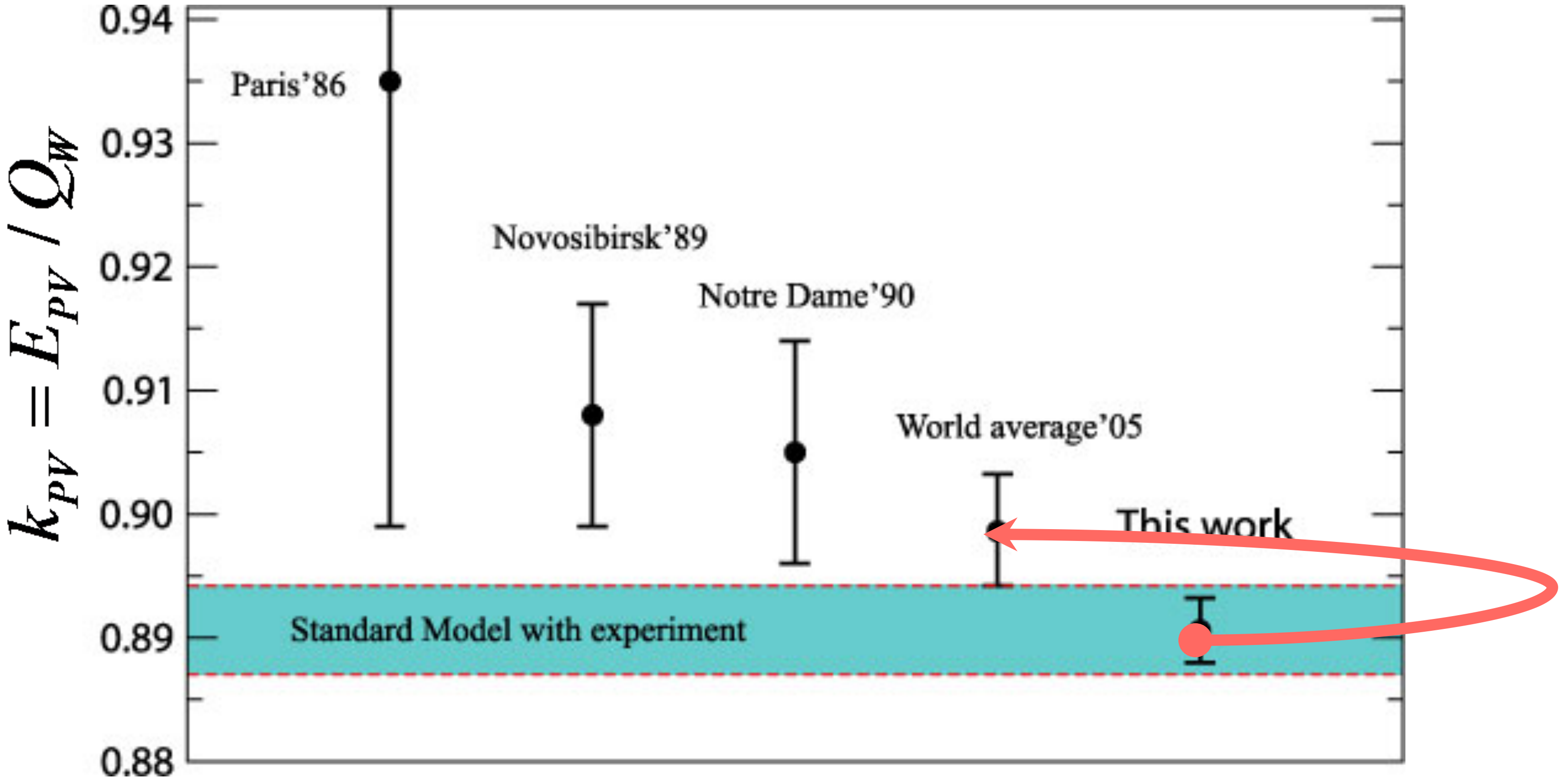
99% of the sum comes from n=6,7,8,9 (main term CCSDvT)

PV Amplitude (2012)

Coulomb interaction		Dzuba *et al* (2012)
Main ($n = 6 - 9$)	0.8823(18)	
Tail	0.0175(18)	→ **0.0256(36)**
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)	→ **0.8977 (40)**

- 2 sigma shift in the tail contribution
- Increase in the error bar ☹
- Total error is dominated by the error in the "tail"
- Technical problem: summation must be over complete set of many-body states: Sydney basis is not the same as ours used for the "Main" term
- Possible solution: CC method in the parity-mixed basis

Theoretical progress (2012)



Lessons on estimating theoretical errors

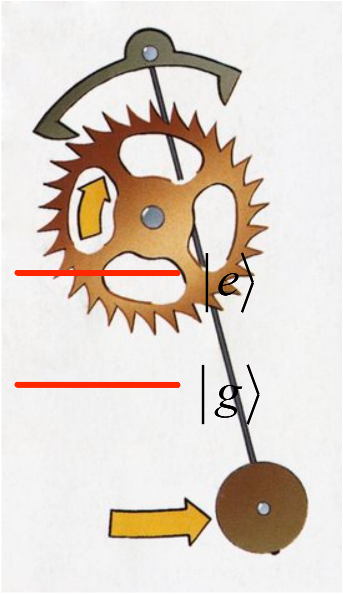
- ☐ Enormous Hilbert space ----> no exact solutions:
  High-accuracy experimental data points is a must (energies, lifetimes, HFS constants, …)
- ☐ Self-consistency checks (e.g. different gauges)
- ☐ Fits to high-accuracy experimental values to estimate missing higher-order effects
- ☐ Numerical error: Basis saturation tests
- ☐ Checks for simple systems where method is exact
- ☐ Blind test
- ☐ Quality control – use symbolic tools for repetitive tasks/coding and deriving diagrams
- ☐ Competing groups – independent tests – complementary techniques help

Atomic parity violation: future experiments

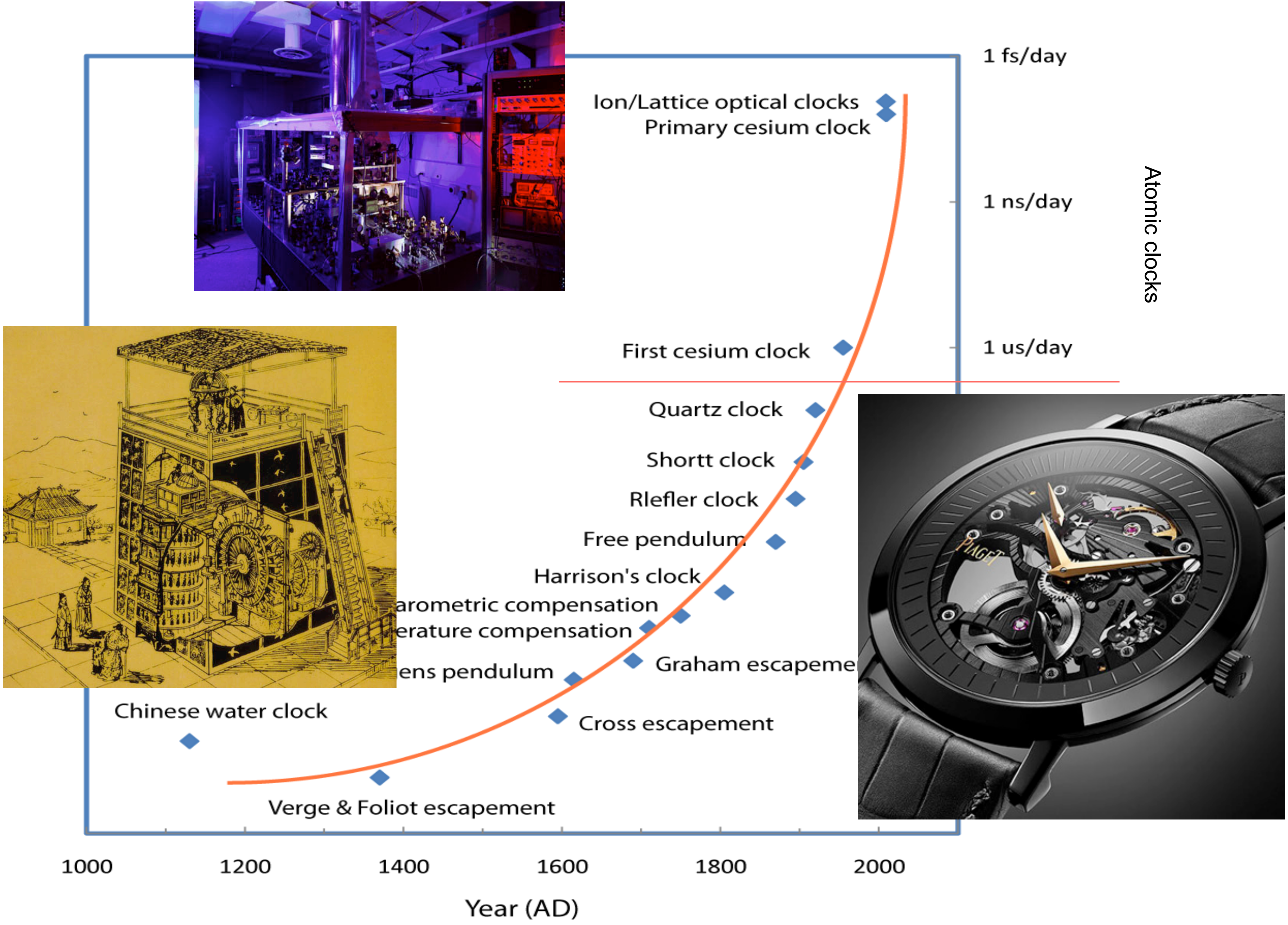
- Cs refined (Dan Elliot - Purdue)
- Dy (Berkeley)
- Fr (TRIUMF-Canada [Maryland/Manitoba/Willam&Mary/San Luis Potosi])
- Ra+ (KVI/the Netherlands)
- Hg (Greece)

Part II:

Nuclear clock and variation of fundamental constants

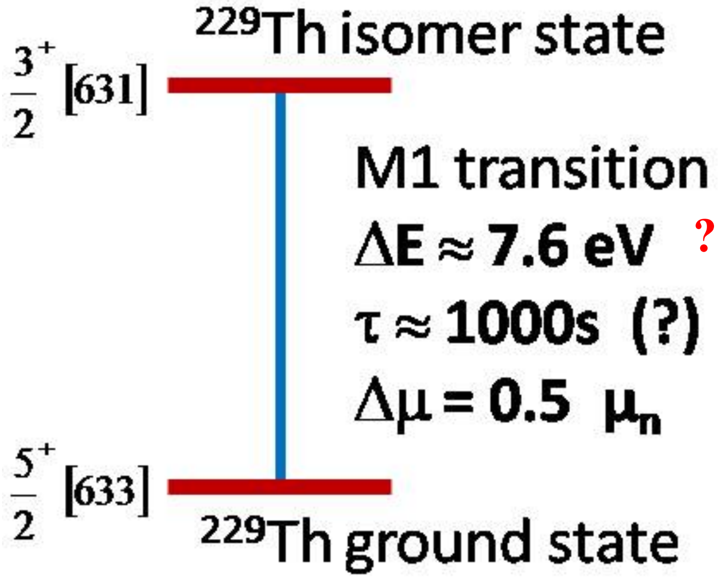


$$\nu_{\text{clock}} = \frac{E_e - E_g}{h}$$


1 fs/day
1 ns/day
1 us/day
Atomic clocks
Ion/Lattice optical clocks
Primary cesium clock
First cesium clock
Quartz clock
Shortt clock
Rlefler clock
Free pendulum
Harrison's clock
arometric compensation
erature compensation
ens pendulum
Graham escapeme
Chinese water clock
Cross escapement
Verge & Foliot escapement
PIAGET
1000
1200
1400
1600
1800
2000
Year (AD)

Shrink the quantum oscillator size ==>
reduced couplings to external perturbations ==>
better accuracy

Nuclear clock



^{229}Th isomer state

$\frac{3}{2}^+$ [631]

M1 transition

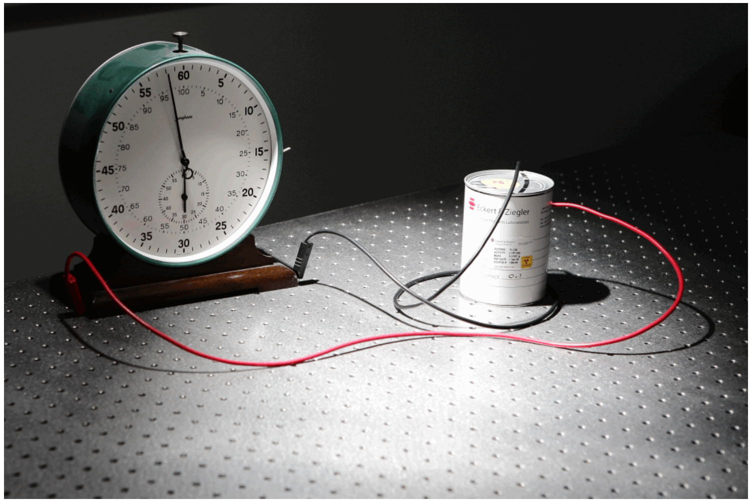
$\Delta E \approx 7.6$ eV ?????

$\tau \approx 1000$s (?)

$\Delta\mu = 0.5\ \mu_n$

$\frac{5}{2}^+$ [633]

^{229}Th ground state



www.thorium.at

Two directions:

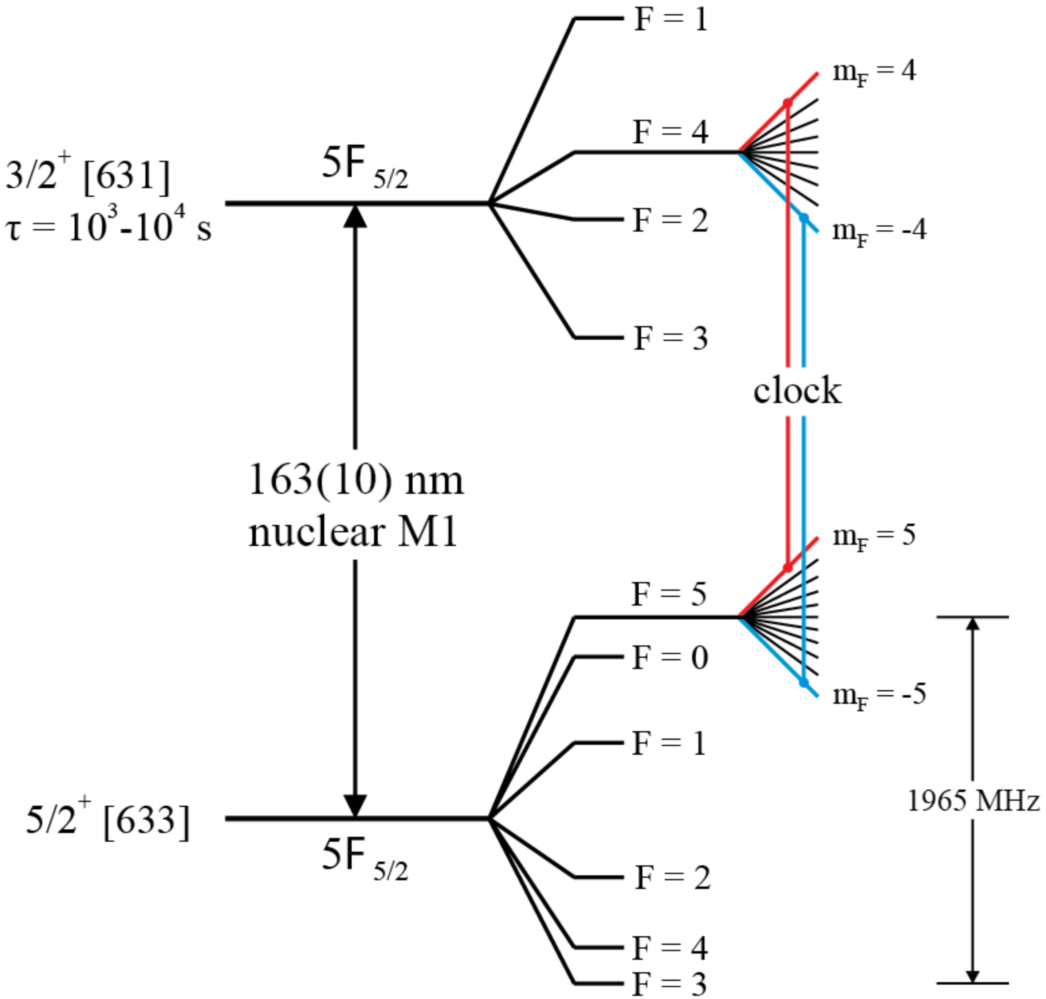
- **Solid state devices with 10^{10} Th nuclei => high-stability (not so accurate)**
- **Ion clocks => high accuracy (not so stable)**

E. Peik and Chr. Tamm, Europhys. Lett. 61, 181 (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)



Uncertainty budget

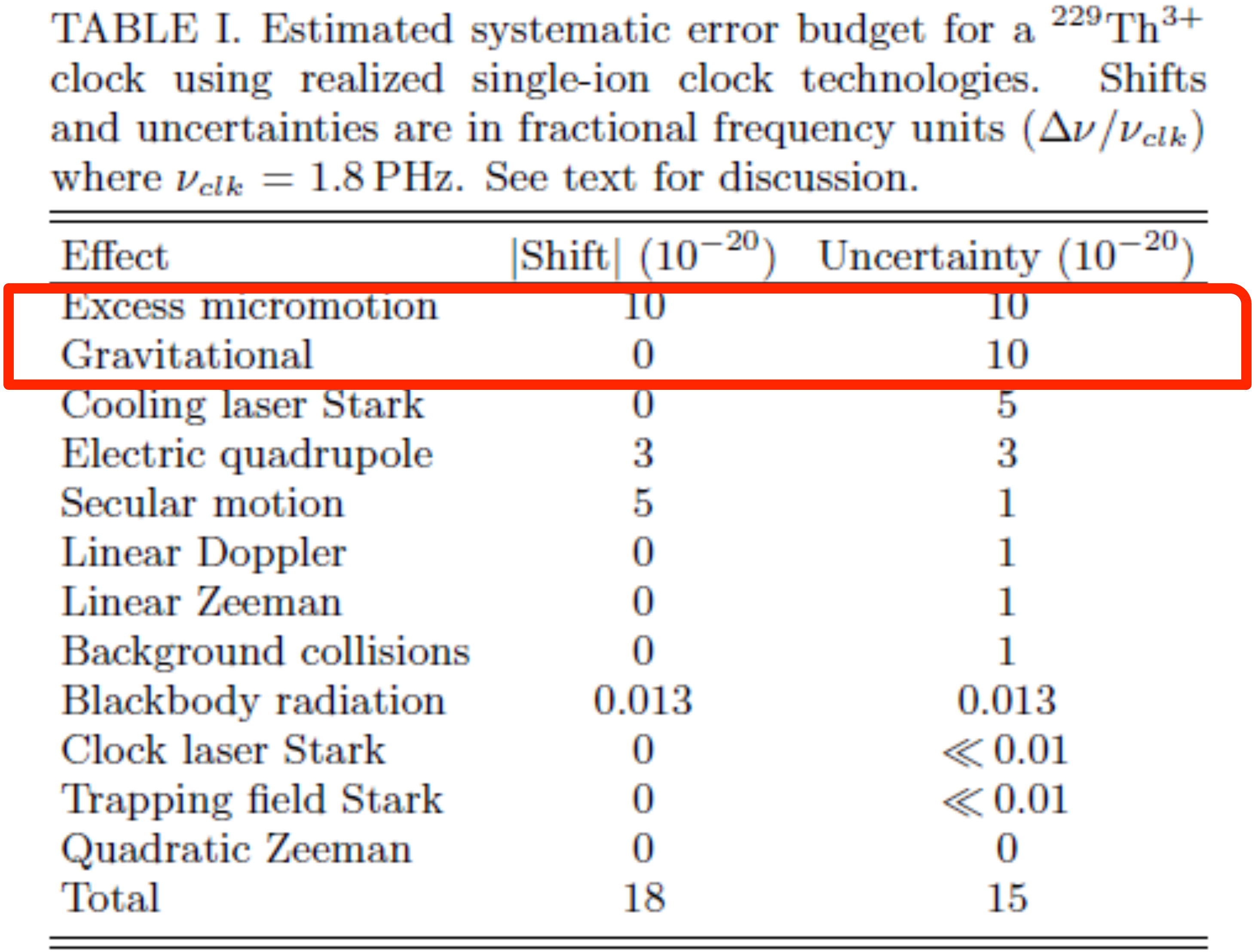


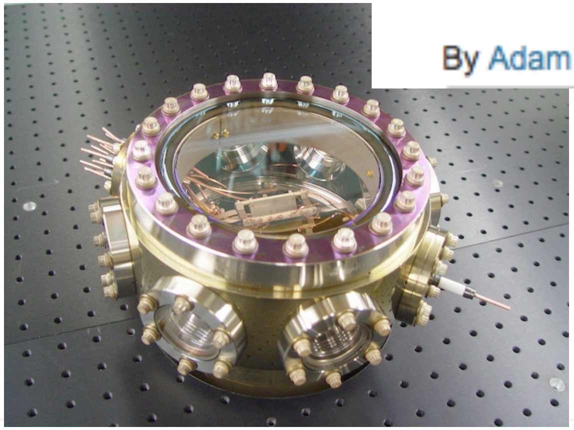
TABLE I. Estimated systematic error budget for a $^{229}\mathrm{Th}^{3+}$ clock using realized single-ion clock technologies. Shifts and uncertainties are in fractional frequency units ($\Delta\nu/\nu_{clk}$) where $\nu_{clk} = 1.8\,\mathrm{PHz}$. See text for discussion.

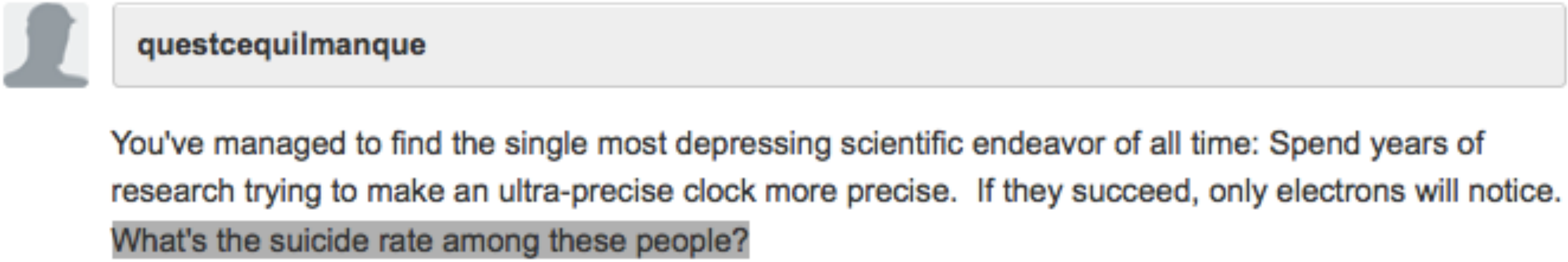
Effect	$\lvert\text{Shift}\rvert$ (10^{-20})	Uncertainty (10^{-20})
Excess micromotion	10	10
Gravitational	0	10
Cooling laser Stark	0	5
Electric quadrupole	3	3
Secular motion	5	1
Linear Doppler	0	1
Linear Zeeman	0	1
Background collisions	0	1
Blackbody radiation	0.013	0.013
Clock laser Stark	0	$\ll 0.01$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

WIRED

Laser-Tuned Nuclear Clock Would Be Accurate for Billions of Years

By Adam Mann ✉ March 20, 2012 | 5:28 pm | Categories: Physics





questcequilmanque

You've managed to find the single most depressing scientific endeavor of all time: Spend years of research trying to make an ultra-precise clock more precise. If they succeed, only electrons will notice. What's the suicide rate among these people?

Sensitivity to variation of fundamental constants

Cosmological indications for spatial variation of alpha (dipole)
The Earth moves : d lnα/dt = 10^{-18}/year

Current limit: d lnα/dt < 10^{-17}/year (Al+/Hg+ clock)

Flambaum (2006) : 10^5 enhancement in ^{229}Th

$$\frac{\delta\omega}{\omega} \approx 10^5\left(4\frac{\delta\alpha}{\alpha} + \frac{\delta X_q}{X_q} - 10\frac{\delta X_s}{X_s}\right)\frac{3.5\text{ eV}}{\omega}$$