Петербургский институт ядерной физики

ATOMIC CALCULATIONS FOR STUDIES OF FUNDAMENTAL SYMMETRIES AND ATOMIC CLOCK RESEARCH

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May 17, 2012

Outline

1. Atomic parity violation

- Present status
- Implications for high-energy and nuclear physics
- Future prospects

2. High-precision atomic methodologies

- Coupled-cluster method for monovalent systems
- Development of hybrid configuration interaction + coupled - cluster approach

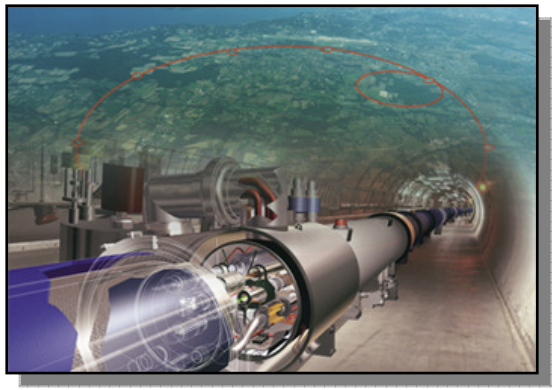
3. Applications to atomic clocks – BBR shifts

4. Tl EDM enhancement factor controversy

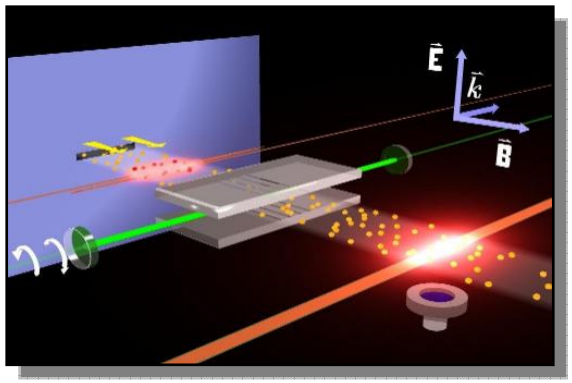
Atomic Parity Violation

High energies

Instead of search for new processes or particles directly



Determine weak charge Q_W from atomic parity violation studies and compare the result with Standard Model prediction

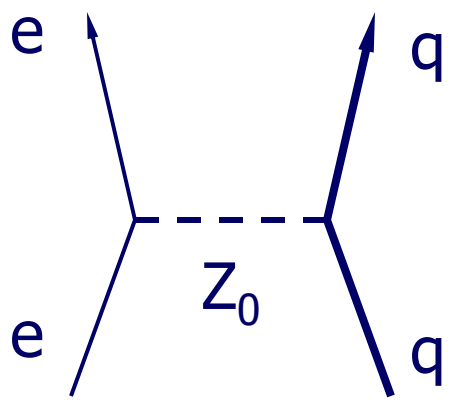


Low energies

http://public.web.cern.ch/, Cs experiment, University of Colorado

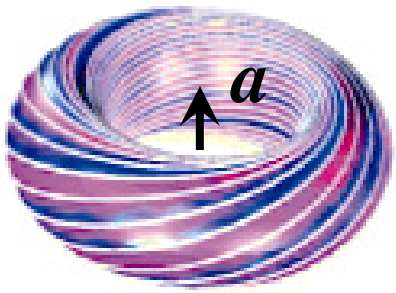
Two sides of the atomic parity violation

NUCLEAR
SPIN-INDEPENDENT
PNC:
SEARCHES FOR NEW
PHYSICS
BEYOND THE
STANDARD MODEL



Weak Charge Q_W

NUCLEAR
SPIN-DEPENDENT
PNC:
STUDY OF PNC
IN THE NUCLEUS



Nuclear anapole moment

EXPERIMENTAL PNC STUDIES

PERIODIC TABLE

Atomic Properties of the Elements

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

Physics Laboratory
physics.nist.gov

Standard Reference Data Group
www.nist.gov/srd

- Solids
- Liquids
- Gases
- Artificially Prepared

Period	Group 1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 $^2S_{1/2}$ **H** Hydrogen 1.00794 1s 13.5984																	2 $^1S_0$ **He** Helium 4.002602 $1s^2$ 24.5874
2	3 $^2S_{1/2}$ **Li** Lithium 6.941 $1s^22s$ 5.3917	4 $^1S_0$ **Be** Beryllium 9.012182 $1s^22s^2$ 9.3227											5 $^2P^\circ_{1/2}$ **B** Boron 10.811 $1s^22s^22p$ 8.2980	6 $^3P_0$ **C** Carbon 12.0107 $1s^22s^22p^2$ 11.2603	7 $^4S^\circ_{3/2}$ **N** Nitrogen 14.0067 $1s^22s^22p^3$ 14.5341	8 $^3P_2$ **O** Oxygen 15.9994 $1s^22s^22p^4$ 13.6181	9 $^2P^\circ_{3/2}$ **F** Fluorine 18.9984032 $1s^22s^22p^5$ 17.4228	10 $^1S_0$ **Ne** Neon 20.1797 $1s^22s^22p^6$ 21.5645
3	11 $^2S_{1/2}$ **Na** Sodium 22.989770 [Ne]3s 5.1391	12 $^1S_0$ **Mg** Magnesium 24.3050 $[Ne]3s^2$ 7.6462											13 $^2P^\circ_{1/2}$ **Al** Aluminum 26.981538 $[Ne]3s^23p$ 5.9858	14 $^3P_0$ **Si** Silicon 28.0855 $[Ne]3s^23p^2$ 8.1517	15 $^4S^\circ_{3/2}$ **P** Phosphorus 30.973761 $[Ne]3s^23p^3$ 10.4867	16 $^3P_2$ **S** Sulfur 32.065 $[Ne]3s^23p^4$ 10.3600	17 $^2P^\circ_{3/2}$ **Cl** Chlorine 35.453 $[Ne]3s^23p^5$ 12.9676	18 $^1S_0$ **Ar** Argon 39.948 $[Ne]3s^23p^6$ 15.7596
4	19 $^2S_{1/2}$ **K** Potassium 39.0983 [Ar]4s 4.3407	20 $^1S_0$ **Ca** Calcium 40.078 $[Ar]4s^2$ 6.1132	21 $^2D_{3/2}$ **Sc** Scandium 44.955910 $[Ar]3d4s^2$ 6.5615	22 $^3F_2$ **Ti** Titanium 47.867 $[Ar]3d^24s^2$ 6.8281	23 $^4F_{3/2}$ **V** Vanadium 50.9415 $[Ar]3d^34s^2$ 6.7462	24 $^7S_3$ **Cr** Chromium 51.9961 $[Ar]3d^54s$ 6.7665	25 $^6S_{5/2}$ **Mn** Manganese 54.938049 $[Ar]3d^54s^2$ 7.4340	26 $^5D_4$ **Fe** Iron 55.845 $[Ar]3d^64s^2$ 7.9024	27 $^4F_{9/2}$ **Co** Cobalt 58.933200 $[Ar]3d^74s^2$ 7.8810	28 $^3F_4$ **Ni** Nickel 58.6934 $[Ar]3d^84s^2$ 7.6398	29 $^2S_{1/2}$ **Cu** Copper 63.546 $[Ar]3d^{10}4s$ 7.7264	30 $^1S_0$ **Zn** Zinc 65.409 $[Ar]3d^{10}4s^2$ 9.3942	31 $^2P^\circ_{1/2}$ **Ga** Gallium 69.723 $[Ar]3d^{10}4s^24p$ 5.9993	32 $^3P_0$ **Ge** Germanium 72.64 $[Ar]3d^{10}4s^24p^2$ 7.8994	33 $^4S^\circ_{3/2}$ **As** Arsenic 74.92160 $[Ar]3d^{10}4s^24p^3$ 9.7886	34 $^3P_2$ **Se** Selenium 78.96 $[Ar]3d^{10}4s^24p^4$ 9.7524	35 $^2P^\circ_{3/2}$ **Br** Bromine 79.904 $[Ar]3d^{10}4s^24p^5$ 11.8138	36 $^1S_0$ **Kr** Krypton 83.798 $[Ar]3d^{10}4s^24p^6$ 13.9996
5	37 $^2S_{1/2}$ **Rb** Rubidium 85.4678 [Kr]5s 4.1771	38 $^1S_0$ **Sr** Strontium 87.62 $[Kr]5s^2$ 5.6949	39 $^2D_{3/2}$ **Y** Yttrium 88.90585 $[Kr]4d5s^2$ 6.2173	40 $^3F_2$ **Zr** Zirconium 91.224 $[Kr]4d^25s^2$ 6.6339	41 $^6D_{1/2}$ **Nb** Niobium 92.90638 $[Kr]4d^45s$ 6.7589	42 $^7S_3$ **Mo** Molybdenum 95.94 $[Kr]4d^55s$ 7.0924	43 $^6S_{5/2}$ **Tc** Technetium (98) $[Kr]4d^55s^2$ 7.28	44 $^5F_5$ **Ru** Ruthenium 101.07 $[Kr]4d^75s$ 7.3605	45 $^4F_{9/2}$ **Rh** Rhodium 102.90550 $[Kr]4d^85s$ 7.4589	46 $^1S_0$ **Pd** Palladium 106.42 $[Kr]4d^{10}$ 8.3369	47 $^2S_{1/2}$ **Ag** Silver 107.8682 $[Kr]4d^{10}5s$ 7.5762	48 $^1S_0$ **Cd** Cadmium 112.411 $[Kr]4d^{10}5s^2$ 8.9938	49 $^2P^\circ_{1/2}$ **In** Indium 114.818 $[Kr]4d^{10}5s^25p$ 5.7864	50 $^3P_0$ **Sn** Tin 118.710 $[Kr]4d^{10}5s^25p^2$ 7.3439	51 $^4S^\circ_{3/2}$ **Sb** Antimony 121.760 $[Kr]4d^{10}5s^25p^3$ 8.6084	52 $^3P_2$ **Te** Tellurium 127.60 $[Kr]4d^{10}5s^25p^4$ 9.0095	53 $^2P^\circ_{3/2}$ **I** Iodine 126.90447 $[Kr]4d^{10}5s^25p^5$ 10.4513	54 $^1S_0$ **Xe** Xenon 131.293 $[Kr]4d^{10}5s^25p^6$ 12.1298
6	55 $^2S_{1/2}$ **Cs** Cesium 132.90545 [Xe]6s 3.8939	56 $^1S_0$ **Ba** Barium 137.327 $[Xe]6s^2$ 5.2117		72 $^3F_2$ **Hf** Hafnium 178.49 $[Xe]4f^{14}5d^26s^2$ 6.8251	73 $^4F_{3/2}$ **Ta** Tantalum 180.9479 $[Xe]4f^{14}5d^36s^2$ 7.5496	74 $^5D_0$ **W** Tungsten 183.84 $[Xe]4f^{14}5d^46s^2$ 7.8640	75 $^6S_{5/2}$ **Re** Rhenium 186.207 $[Xe]4f^{14}5d^56s^2$ 7.8335	76 $^5D_4$ **Os** Osmium 190.23 $[Xe]4f^{14}5d^66s^2$ 8.4382	77 $^4F_{9/2}$ **Ir** Iridium 192.217 $[Xe]4f^{14}5d^76s^2$ 8.9670	78 $^3D_3$ **Pt** Platinum 195.078 $[Xe]4f^{14}5d^96s$ 8.9588	79 $^2S_{1/2}$ **Au** Gold 196.96655 $[Xe]4f^{14}5d^{10}6s$ 9.2255	80 $^1S_0$ **Hg** Mercury 200.59 $[Xe]4f^{14}5d^{10}6s^2$ 10.4375	81 $^2P^\circ_{1/2}$ **Tl** Thallium 204.3833 [Hg]6p 6.1082	82 $^3P_0$ **Pb** Lead 207.2 $[Hg]6p^2$ 7.4167	83 $^4S^\circ_{3/2}$ **Bi** Bismuth 208.98038 $[Hg]6p^3$ 7.2855	84 $^3P_2$ **Po** Polonium (209) $[Hg]6p^4$ 8.414	85 $^2P^\circ_{3/2}$ **At** Astatine (210) $[Hg]6p^5$	86 $^1S_0$ **Rn** Radon (222) $[Hg]6p^6$ 10.7485
7	87 $^2S_{1/2}$ **Fr** Francium (223) [Rn]7s 4.0727	88 $^1S_0$ **Ra** Radium (226) $[Rn]7s^2$ 5.2784		104 $^3F_2$? **Rf** Rutherfordium (261) $[Rn]5f^{14}6d^27s^2$? 6.0 ?	105 **Db** Dubnium (262)	106 **Sg** Seaborgium (266)	107 **Bh** Bohrium (264)	108 **Hs** Hassium (277)	109 **Mt** Meitnerium (268)	110 **Uun** Ununnilium (281)	111 **Uuu** Unununium (272)	112 **Uub** Ununbium (285)		114 **Uuq** Ununquadium (289)		116 **Uuh** Ununhexium (292)		

Lanthanides	57 $^2D_{3/2}$ **La** Lanthanum 138.9055 $[Xe]5d6s^2$ 5.5769	58 $^1G^\circ_4$ **Ce** Cerium 140.116 $[Xe]4f5d6s^2$ 5.5387	59 $^4I^\circ_{9/2}$ **Pr** Praseodymium 140.90765 $[Xe]4f^36s^2$ 5.473	60 $^5I_4$ **Nd** Neodymium 144.24 $[Xe]4f^46s^2$ 5.5250	61 $^6H^\circ_{5/2}$ **Pm** Promethium (145) $[Xe]4f^56s^2$ 5.582	62 $^7F_0$ **Sm** Samarium 150.36 $[Xe]4f^66s^2$ 5.6437	63 $^8S^\circ_{7/2}$ **Eu** Europium 151.964 $[Xe]4f^76s^2$ 5.6704	64 $^9D^\circ_2$ **Gd** Gadolinium 157.25 $[Xe]4f^75d6s^2$ 6.1498	65 $^6H^\circ_{15/2}$ **Tb** Terbium 158.92534 $[Xe]4f^96s^2$ 5.8638	66 $^5I_8$ **Dy** Dysprosium 162.500 $[Xe]4f^{10}6s^2$ 5.9389	67 $^4I^\circ_{15/2}$ **Ho** Holmium 164.93032 $[Xe]4f^{11}6s^2$ 6.0215	68 $^3H_6$ **Er** Erbium 167.259 $[Xe]4f^{12}6s^2$ 6.1077	69 $^2F^\circ_{7/2}$ **Tm** Thulium 168.93421 $[Xe]4f^{13}6s^2$ 6.1843	70 $^1S_0$ **Yb** Ytterbium 173.04 $[Xe]4f^{14}6s^2$ 6.2542	71 $^2D_{3/2}$ **Lu** Lutetium 174.967 $[Xe]4f^{14}5d6s^2$ 5.4259
Actinides	89 $^2D_{3/2}$ **Ac** Actinium (227) $[Rn]6d7s^2$ 5.17	90 $^3F_2$ **Th** Thorium 232.0381 $[Rn]6d^27s^2$ 6.3067	91 $^4K_{11/2}$ **Pa** Protactinium 231.03588 $[Rn]5f^26d7s^2$ 5.89	92 $^5L^\circ_6$ **U** Uranium 238.02891 $[Rn]5f^36d7s^2$ 6.1941	93 $^6L_{11/2}$ **Np** Neptunium (237) $[Rn]5f^46d7s^2$ 6.2657	94 $^7F_0$ **Pu** Plutonium (244) $[Rn]5f^67s^2$ 6.0260	95 $^8S^\circ_{7/2}$ **Am** Americium (243) $[Rn]5f^77s^2$ 5.9738	96 $^9D^\circ_2$ **Cm** Curium (247) $[Rn]5f^76d7s^2$ 5.9914	97 $^6H^\circ_{15/2}$ **Bk** Berkelium (247) $[Rn]5f^97s^2$ 6.1979	98 $^5I_8$ **Cf** Californium (251) $[Rn]5f^{10}7s^2$ 6.2817	99 $^4I^\circ_{15/2}$ **Es** Einsteinium (252) $[Rn]5f^{11}7s^2$ 6.42	100 $^3H_6$ **Fm** Fermium (257) $[Rn]5f^{12}7s^2$ 6.50	101 $^2F^\circ_{7/2}$ **Md** Mendelevium (258) $[Rn]5f^{13}7s^2$ 6.58	102 $^1S_0$ **No** Nobelium (259) $[Rn]5f^{14}7s^2$ 6.65	103 $^2P^\circ_{1/2}$? **Lr** Lawrencium (262) $[Rn]5f^{14}7s^27p$? 4.9 ?

Atomic Number — Ground-state Level
Symbol — 58 $^1G^\circ_4$ **Ce**
Name — Cerium
Atomic Weight† — 140.116
Ground-state Configuration — $[Xe]4f5d6s^2$
Ionization Energy (eV) — 5.5387

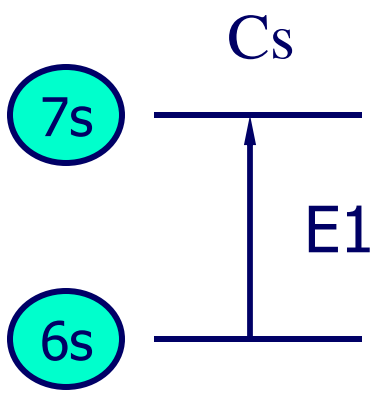
†Based upon ^{12}C. () indicates the mass number of the most stable isotope.

For a description of the data, visit physics.nist.gov/data

NIST SP 966 (September 2003)

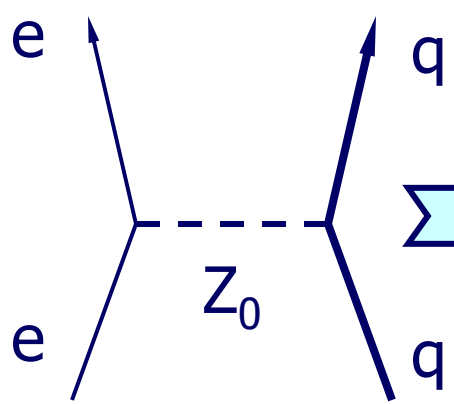
Atomic Parity Violation

$\vec{r} \rightarrow -\vec{r}$



Non-zero transition amplitude
PNC amplitude E_{PNC}

Both 6s and 7s states acquire an opposite-parity ($np_{1/2}$) admixture



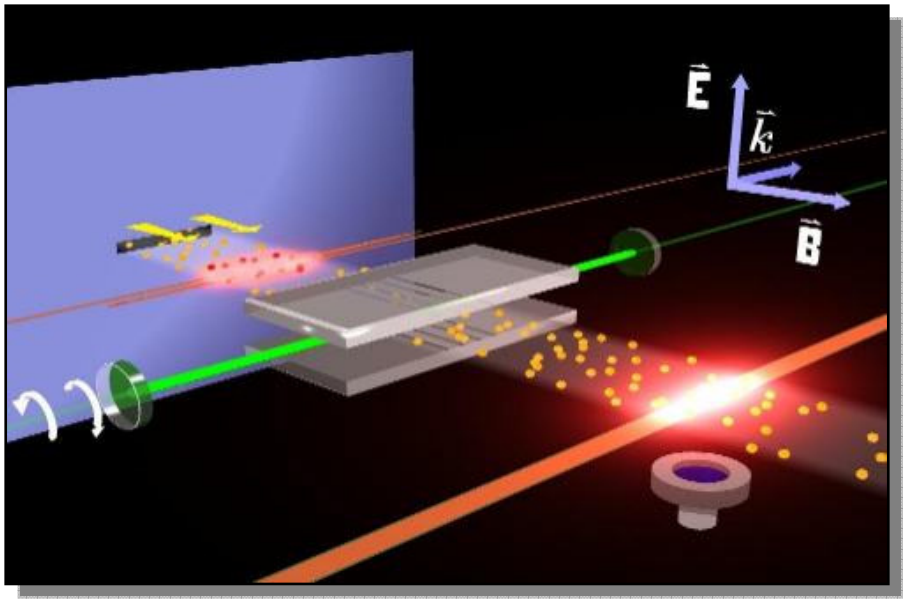
Z_0 exchange: Laporte's rule is violated!

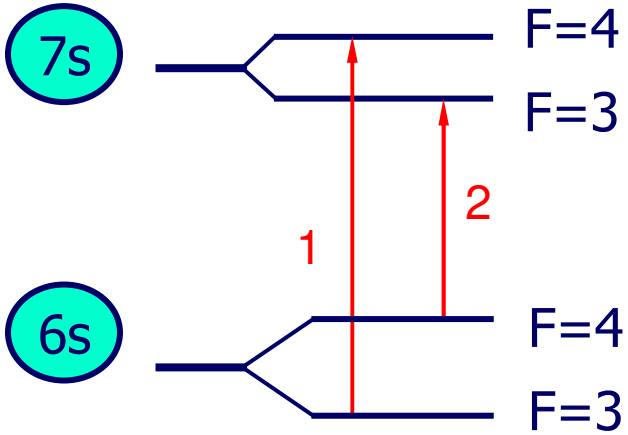
Note: it is really tiny effect !!! E_{PNC} ~**10^{-11}** atomic units

E1 amplitude for 6s – 6p transition is **4.5** atomic units

The most precise measurement of PNC amplitude (cesium)

C.S. Wood et al. Science 275, 1759 (1997)





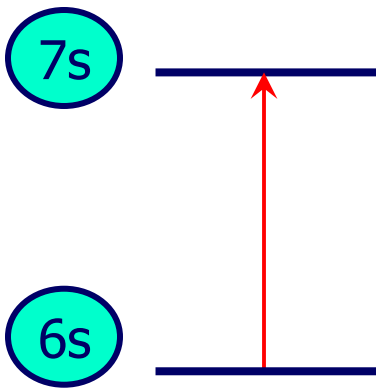
$$\frac{\mathrm{Im}\left(E_{\mathrm{PNC}}\right)}{\beta} = \begin{cases} -1.6349(80)\ \mathrm{mV/cm} & 1 \\ -1.5576(77)\ \mathrm{mV/cm} & 2 \end{cases}$$

0.35% accuracy

Stark interference scheme to measure ratio of the PNC amplitude and the Stark-induced amplitude β

Analysis of Cs PNC experiment

NUCLEAR SPIN-INDEPENDENT PNC

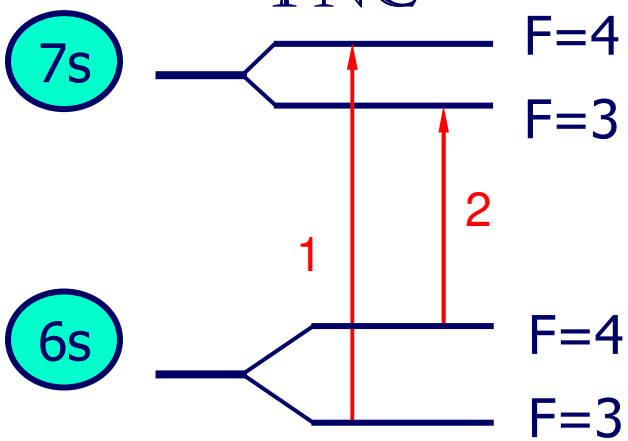


Average of 1 & 2

$$\frac{\mathrm{Im}\left(E_{\mathrm{PNC}}^{\mathrm{si}}\right)}{\beta} = -1.5935(56)\ {}^{\mathrm{mV}}\!/_{\mathrm{cm}}$$

Weak Charge Q_W

NUCLEAR SPIN-DEPENDENT PNC



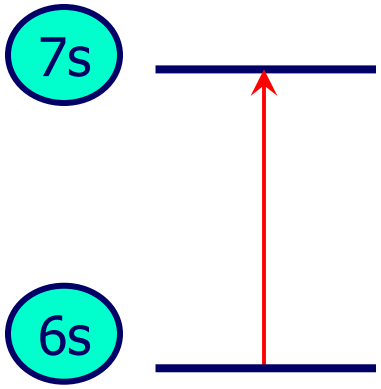
Difference of 1 & 2

$$\Delta\left[\mathrm{Im}\left(E_{\mathrm{PNC}}^{\mathrm{sd}}\right)/\beta\right]_{34-43} = -0.077(11)\ {}^{\mathrm{mV}}\!/_{\mathrm{cm}}$$

Nuclear anapole moment

Analysis of Cs PNC experiment

NUCLEAR
SPIN-INDEPENDENT
PNC

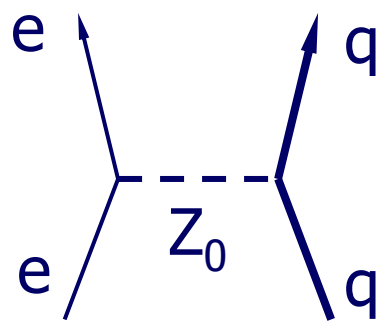


Average of 1 & 2

$$\frac{\mathrm{Im}\left(E_{\mathrm{PNC}}^{\mathrm{si}}\right)}{\beta} = -1.5935(56)\ {}^{\mathrm{mV}}\!/_{\mathrm{cm}}$$

Weak Charge Q_W

How to extract weak charge Q_w from Cs experiment?



Electron-quark parity violating interaction (exchange of virtual Z_0 boson)

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

Neutron density function

Electronic sector: $$H^{(1)}_{PNC} = \frac{G_F}{2\sqrt{2}} Q_W \gamma_5 \rho(r)$$

Extraction of weak the charge:

Theoretical calculation of PNC amplitude

Measured value $\longrightarrow$ $$E_{PNC} = E^{theory}_{PNC} Q_W^{\text{inferred}}$$

Calculation of PNC amplitude

1. Main part – Coulomb interactions

Electric-dipole matrix elements

$$E_{\mathrm{PNC}}^{theory} = \sum_{n=2}^{\infty} \frac{\langle 7s|d|np_{1/2}\rangle\langle np_{1/2}|H_{\mathrm{PNC}}|6s\rangle}{E_{6s} - E_{np_{1/2}}} + \sum_{n=2}^{\infty} \frac{\langle 7s|H_{\mathrm{PNC}}|np_{1/2}\rangle\langle np_{1/2}|d|6s\rangle}{E_{7s} - E_{np_{1/2}}}$$

Energies

PNC matrix elements

Sum is separated to main part, n = 6 - 9 and the tail

2. Other small corrections:

Breit, QED, Neutron skin, e – e weak interaction

Cs PNC: Comparison with the standard model

Standard Model [1] : $$Q_W^{\mathrm{SM}} = -73.16(3)$$

Most current result for Cs PNC Expt/Theory:

Atomic physics [2] :

$$Q_W^{\mathrm{inferred}} = -73.16(29)_{\mathrm{expt}}(20)_{\mathrm{theory}}$$

No deviation from the Standard Model

[1] C. Amsler et al. (Partical Data Group), Phys. Lett. B 667, 1 (2008)
[2] S. G. Porsev, K. Beloy and A. Derevianko, PRL 102, 181601 (2009), Phys. Rev. D **82**, 036008 (2010)

IMPLICATIONS FOR PARTICLE PHYSICS

Confirms fundamental "running" (energy dependence) of the electroweak force over energy span 10 MeV → 100 GeV

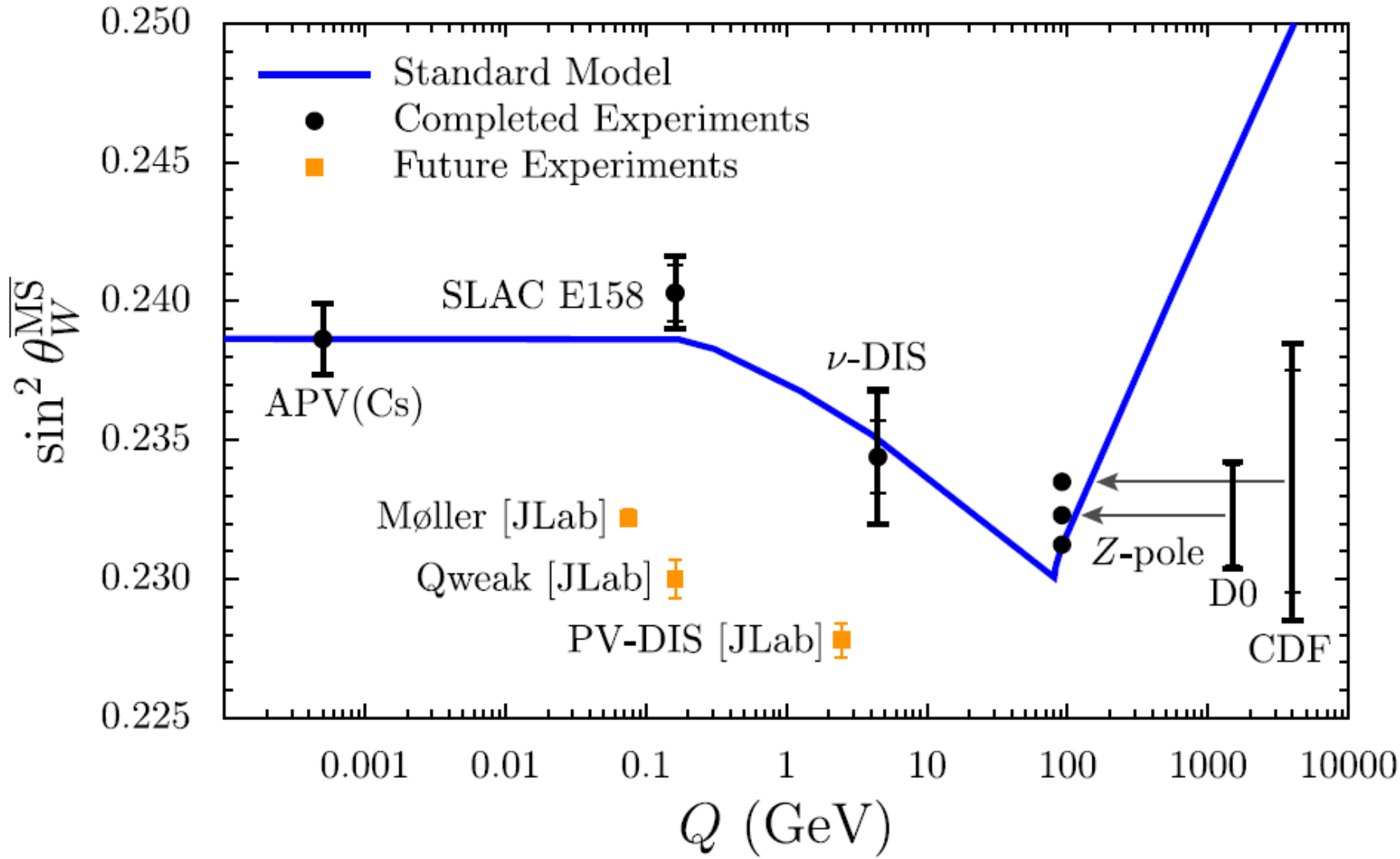


Figure is from Bentz *et al. Phys. Lett.* ***B693***, 462 (2010).

Probing new physics

New physics can be phenomenologically described by weak isospin - conserving S and isospin - breaking T parameters [1].

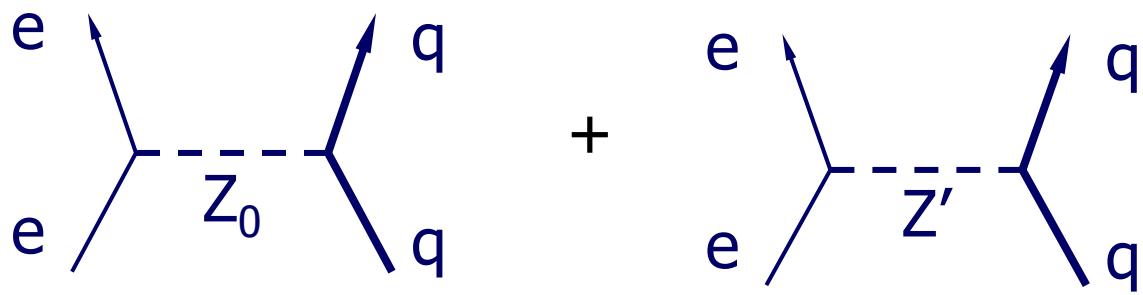
$$\Delta Q = Q_W^{\text{inferred}} - Q_W^{\text{SM}} = -0.800S - 0.007T$$

Present result [2]: $|S| < 0.45$

Parameter S is important for indirect constraint on the mass of Higgs particle [1].

[1] J.L. Rosner, PRD 65, 073026 (2002)
[2] S. G. Porsev, K. Beloy and A. Derevianko, PRL 102, 181601 (2009), Phys. Rev. D **82**, 036008 (2010)

Probing new physics: extra Z bosons



Atomic parity violation is uniquely sensitive to Z′

Z'_χ in SO(10) GUT, Marciano & Rosner

$$\Delta Q = Q_W^{\text{inferred}} - Q_W^{\text{SM}} \approx \left(\frac{0.736\ \text{TeV}/c^2}{M_{Z'_x}} \right)^2$$

Probing new physics: extra Z bosons

Z'_X in SO(10) GUT, Marciano & Rosner

$$\Delta Q = Q_W^{\text{inferred}} - Q_W^{\text{SM}} \approx \left(\frac{0.736\ \text{TeV}/c^2}{M_{Z'_x}} \right)^2$$

Cs result [1] implies $M_{Z'_x} > 1.3\text{TeV}/c^2$

Direct search at Tevatron collider [2]

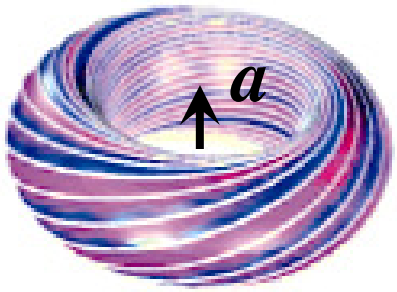
$$M_{Z'_x} > 0.82\text{TeV}/c^2$$

[1] S. G. Porsev, K. Beloy and A. Derevianko, PRL 102, 181601 (2009)
[2] T. Aaltonen et al., Phys. Rev. Lett. 99, 171802 (2007)

Parity violation in atoms

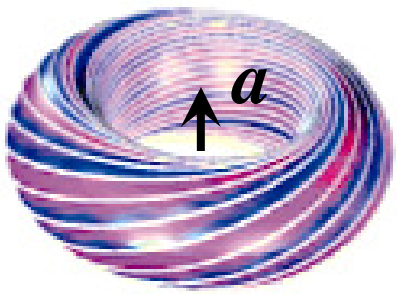
The other part of the story

NUCLEAR
SPIN-DEPENDENT
PNC:
STUDY OF PNC
IN THE NUCLEUS



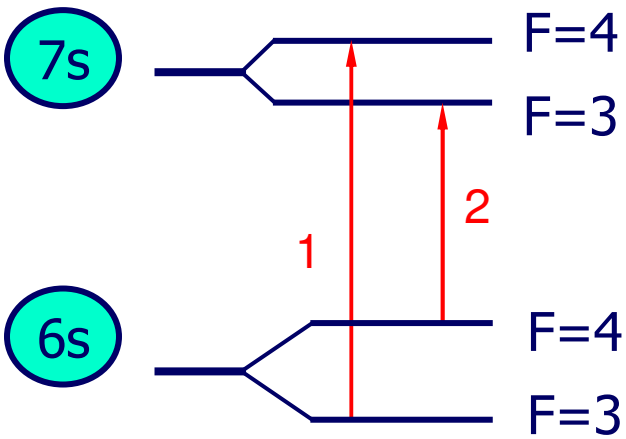
Nuclear anapole moment

Spin-dependent parity violation: Nuclear anapole moment



Parity-violating nuclear moment

Valence nucleon density

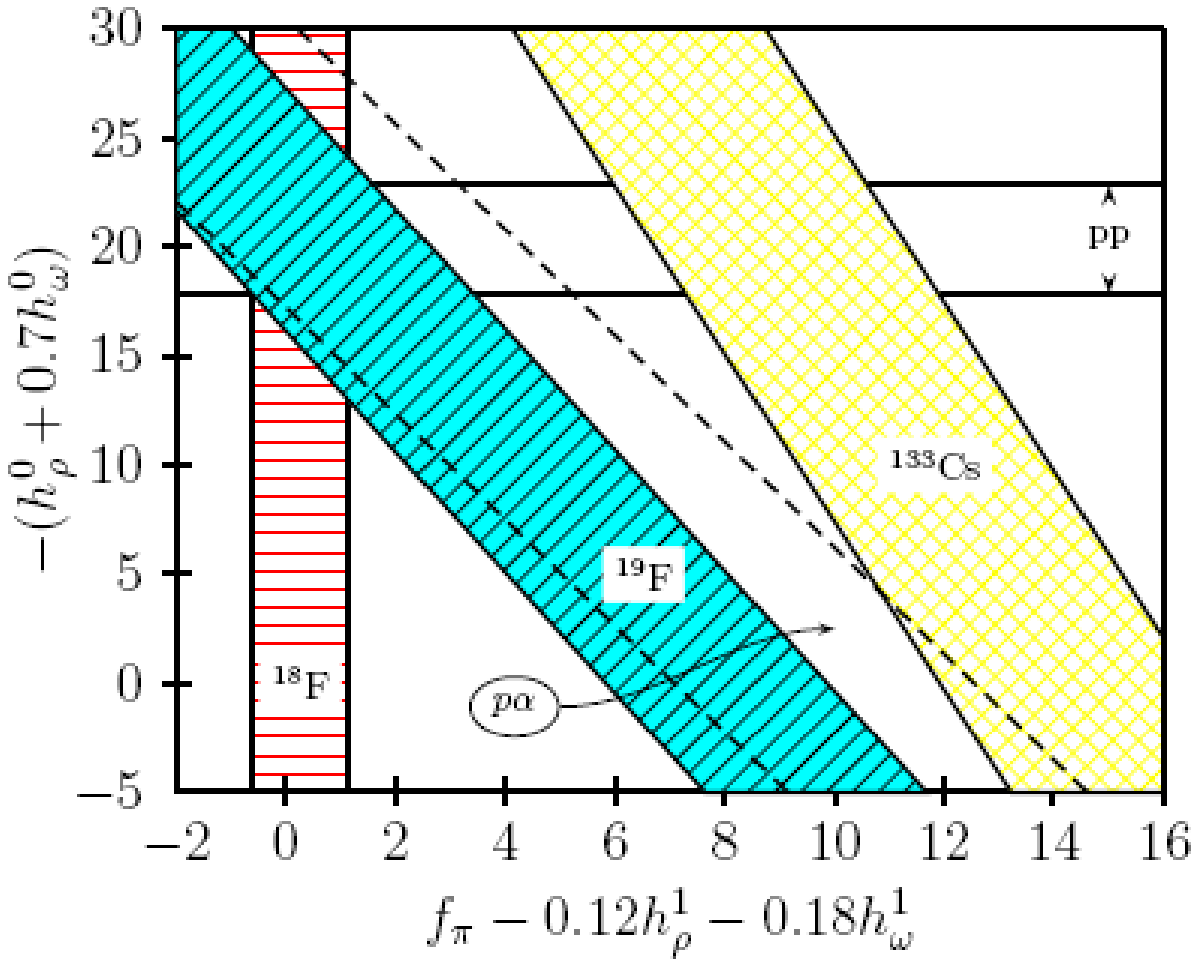


$$H_{\mathrm{PNC}}^{(\mathrm{a})} = \frac{G_F}{\sqrt{2}} \kappa_a \, \boldsymbol{\alpha} \cdot \mathbf{I} \;\; \rho_v(r)$$

Anapole moment

Nuclear anapole moment is parity-odd, time-reversal-even E1 moment of the electromagnetic current operator.

Constraints on nuclear weak coupling contants



W. C. Haxton and C. E. Wieman, Ann. Rev. Nucl. Part. Sci. 51, 261 (2001)

Nuclear anapole moment?

The constraints obtained from the Cs experiment were found to be ***inconsistent*** with constraints from other nuclear PNC measurements, which favor a smaller value of the ^{133}Cs anapole moment.

Possible atomic calculation solution?

$\kappa = 0.117(16)$

Incomplete correlation calculation of spin-dependent PNC amplitude?

Nuclear anapole moment: Test of hadronic weak interations

The constraints obtained from the Cs experiment were found to be inconsistent with constraints from other nuclear PNC measurements, which favor a smaller value of the ^{133}Cs anapole moment.

All-order (LCCSD) calculation of spin-dependent PNC amplitude:

k = 0.107(16)* [1% theory accuracy]

No significant difference with previous value k = 0.112(16) is found.

NEED NEW EXPERIMENTS!!!

Fr, Yb, Ra$^+$

*M.S. Safronova, Rupsi Pal, Dansha Jiang, M.G. Kozlov, W.R. Johnson, and U.I. Safronova, Nuclear Physics A 827 (2009) 411c

Summary: Atomic Parity Violation

A: New analysis of atomic PNC experiment is Cs: Nuclear spin-independent part:

(1) Provided most accurate to-date test of the low-energy electroweak sector of the SM.

(2) Confirmed fundamental "running" (energy dependence) of the electroweak force.

(3) Placed constraints are on a variety of new physics scenarios beyond the SM.

B: New analysis of atomic PNC experiment is Cs: Nuclear spin-independent part (anapole moment)

(1) New calculations, accurate to 1% - essentially the same result.

(2) Constraints on nuclear weak coupling constants are still inconsistent with nuclear physics experiments.

NEED NEW EXPERIMENTAL PNC STUDIES

WANTED!

Prospects for Theory Improvement

Fr and Ra^+: 1-3% at present
0.5% possible with CCSDT (same as Cs)

Yb: 9% at present
Significant improvement should be be possible with
CI + coupled-cluster, especially if triples are implemented

Dy: ? Previous: no signal within 2 orders of magnitude from prediction. The problems appears to be somewhat understood at this time. Significant improvement possible if CI+MBPT could be implemented.

Tl, Bi, Pb – improvements to 1% should be possible

2. High-precision atomic methodologies

Summary of Theory Methods for PNC Calculations

- Configuration interaction (CI)
- Many-body perturbation theory
- Relativistic all-order method (coupled-cluster)
- Perturbation theory in the screened Coulomb interaction (PTSCI), all-order approach

- Configuration interaction + second-order MBPT
- Configuration interaction + coupled-cluster method*

*under development

Summary of Theory Methods for PNC Calculations

- Configuration interaction (CI)
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- Configuration interaction + second-order MBPT
- Configuration interaction + coupled-cluster method

Coupled-cluster method (CCSD)

$$\left|\Psi_v\right\rangle = \Omega\left|\Psi_v^{(0)}\right\rangle = \exp(S)\left|\Psi_v^{(0)}\right\rangle$$

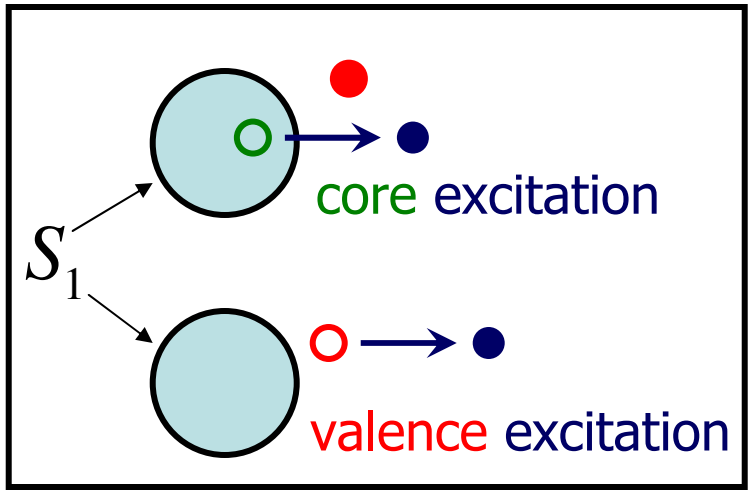
DHF wave function

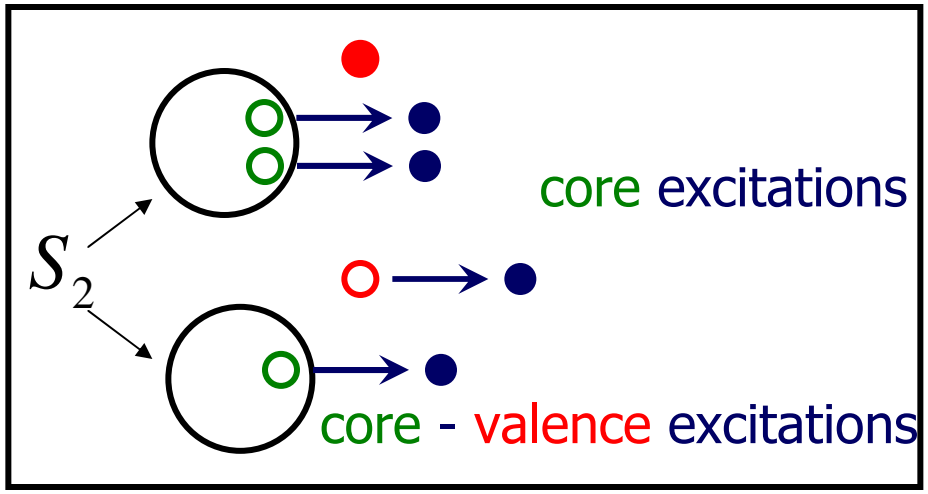
$$\exp(S_1 + S_2)$$

CCSD single-double coupled-cluster

$$S_1 + S_2$$

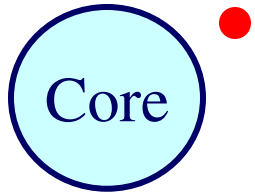
LCCSD coupled-cluster





ALL-ORDER ATOMIC WAVE FUNCTION (SD)

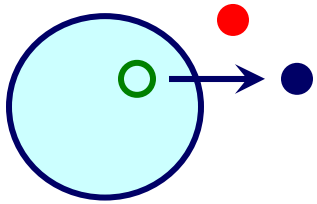
Lowest order



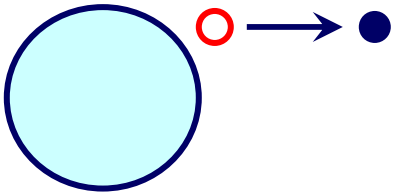
$$\left|\Psi_v^{(0)}\right\rangle$$

core
valence electron
any excited orbital

Single-particle excitations

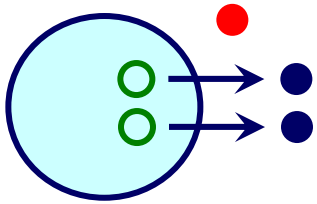


$$\sum_{ma} \rho_{ma}\, a_m^\dagger a_a \left|\Psi_v^{(0)}\right\rangle$$

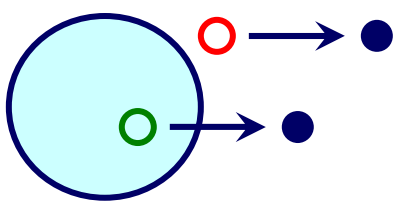


$$\sum_{m\neq v} \rho_{mv}\, a_m^\dagger a_v \left|\Psi_v^{(0)}\right\rangle$$

Double-particle excitations



$$\frac{1}{2}\sum_{mnab} \rho_{mnab}\, a_m^\dagger a_n^\dagger a_b a_a \left|\Psi_v^{(0)}\right\rangle$$



$$\sum_{mna} \rho_{mnva}\, a_m^\dagger a_n^\dagger a_a a_v \left|\Psi_v^{(0)}\right\rangle$$

ALL-ORDER MATRIX ELEMENTS

So we calculated all ρ_{ma}, ρ_{mnab}, ρ_{mv}, ρ_{mnva} .

We now have a really large file with ρ.

How do we calculate matrix elements?

$$Z_{wv} = \frac{\langle \Psi_w | Z_{(E1,E2,PNC,etc.)} | \Psi_v \rangle}{\sqrt{\langle \Psi_w | \Psi_w \rangle \langle \Psi_v | \Psi_v \rangle}}$$

Linear or quadratic functions of excitations coefficients

$$z_{wv}^{(0)} + z^{(a)} + \ldots + z^{(t)}$$

This method works for any one-body operator: ok to calculate E1, E2, E3, M1, M2, PNC, spin-dep. PNC, hyperfine A and B, etc.

Polarizabilities, PNC amplitudes, etc.

Sum-over-states in a finite basis set

Dynamic polarizability:

$$\alpha_v^0(\omega) = \frac{1}{3(2j_v+1)} \sum_n \frac{(E_n - E_v)\left|\langle n \| D \| v \rangle\right|^2}{(E_n - E_v)^2 - \omega^2}$$

PNC amplitude in Cs:

$$E_{\mathrm{PNC}}^{theory} = \sum_{n=2}^{\infty} \frac{\langle 7s | d | np_{1/2} \rangle \langle np_{1/2} | H_{\mathrm{PNC}} | 6s \rangle}{E_{6s} - E_{np_{1/2}}} + \sum_{n=2}^{\infty} \frac{\langle 7s | H_{\mathrm{PNC}} | np_{1/2} \rangle \langle np_{1/2} | d | 6s \rangle}{E_{7s} - E_{np_{1/2}}}$$

Actual implementation

1. Need very accurate (large) basis sets, up to 70x13=910 orbitals

ρ_{mnab} Even with 35 orbitals for each partial wave:

Cs: a,b = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6$

m,n : *finite basis set* = $(35 \times 13) \times (35 \times 13)$

Total actually $15412 \times 35 \times 35 \sim 19\,000\,000$ equations

to be solved iteratively!

Our implementation of the coupled-cluster is different from quantum chemistry – new sets of codes were developed.

Actual implementation

These are really complicated equations !!!

- "Quadruple" term: $\sum_{rs} g_{mnrs} \rho_{rsab}$

a,b core
(17 shells)

Indices $mnrs$ can be **ANY** orbitals

Basis set: n_{max}=**35**, l_{max}=6

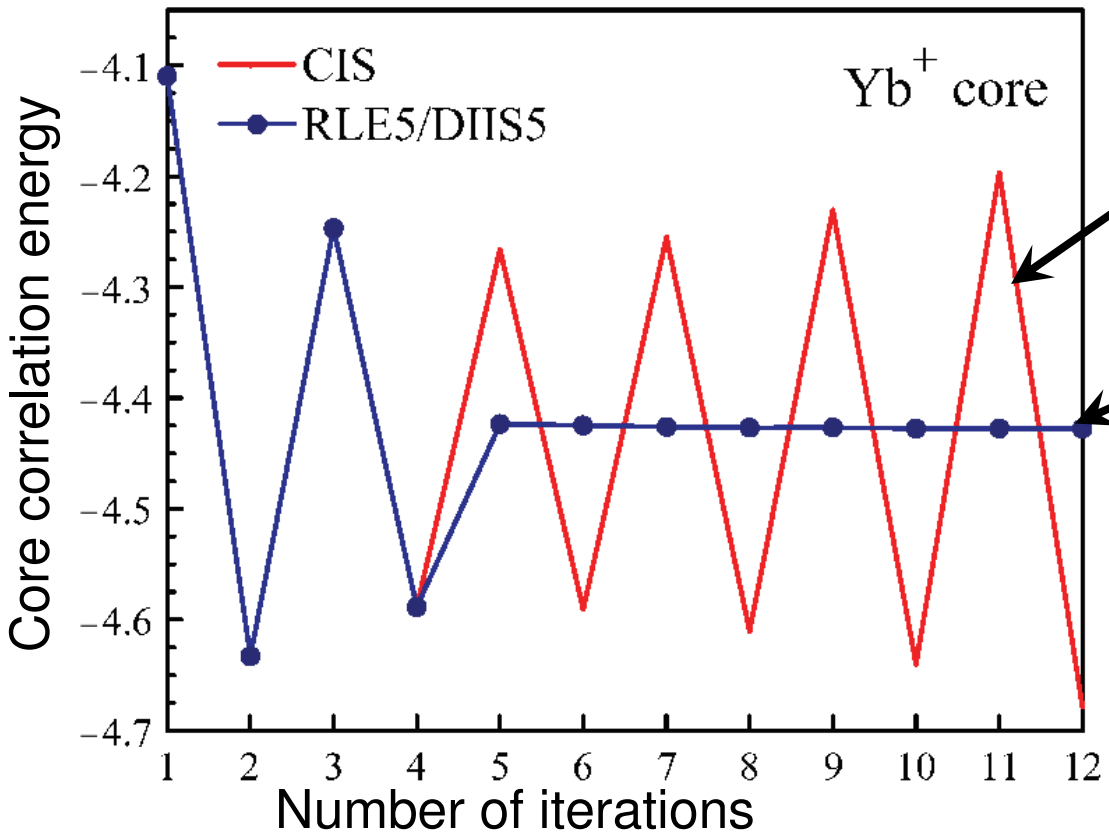
$17 \times 17 \times (35 \times 13)^4 = 5 \times 10^{12}$!

- Program has to be exceptionally efficient!

Actual implementation

Equations for excitation coefficients ρ may diverge!

Example: iterations for Yb^+ core



No stabilizer-equations diverge

With RLE or DIIS stabilizers – problem solved !

H. Gharibnejad, E. Eliav, M.S. Safronova, and A. Derevianko, PRA 83, 052502 (2011)

Extensions of LCCSD

Add more terms to the all order wave-function

Non-linear terms

$$\frac{1}{2}(S_1^2 + 2S_1S_2 + S_2^2)$$

$$+\frac{1}{6}(S_1^3 + 3S_1^2S_2) + \frac{1}{24}S_1^4$$

Triple excitations

$$S_3$$

Non-linear terms

$$\frac{1}{2} S_2^2$$

Contract operators by Wick's theorem

$$H \frac{1}{2} S_2^2 \,|\, \Psi_v^{(0)} > \rightarrow : a_i^+ a_j^+ a_l a_k : a_m^+ a_n^+ a_r^+ a_s^+ a_d a_c a_b a_a a_v^+ : |\, 0_c >$$

Non-linear terms

$$\frac{1}{2} S_2^2$$

Contract operators by Wick's theorem

$$H \frac{1}{2} S_2^2 \,|\, \Psi_v^{(0)} > \rightarrow : a_i^+ a_j^+ a_l a_k : a_m^+ a_n^+ a_r^+ a_s^+ a_d a_c a_b a_a a_v^+ : |\, 0_c >$$

800 TERMS!

Codes that write formulas

The derivation gets **really complicated** if you add triples and non-linear terms!

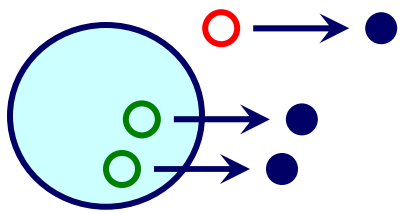
Solution: develop analytical codes that do all the work for you!

Input: ASCII input of terms of the type

$$\sum_{mnrab} \sum_{ijkl} g_{ijkl} \rho_{mnrvab} : a_i^\dagger a_j^\dagger a_l a_k : : a_m^\dagger a_n^\dagger a_r^\dagger a_b a_a a_v : \left| \Psi_v^{(0)} \right\rangle$$

Output: final simplified formula in LATEX to be used in the all-order equation

Triple excitations



- core
- valence electron
- any excited orbital

$$\sum_{mnrab} \rho_{mnrvab}\, a_m^\dagger a_n^\dagger a_r^\dagger a_a a_b a_v \left| \Psi_v^{(0)} \right\rangle$$

Problem 1: too many excitation coefficients ρ_{mnrvab}

Problem 2: increased complexity of equations .

Triple excitations

Problem: too many excitation coefficients ρ_{mnrvab} .

Doubles:

ρ_{mnab}

Cs: a,b = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6$

m,n : *finite basis set* = $(35 \times 13) \times (35 \times 13)$

Smallest required basis set:

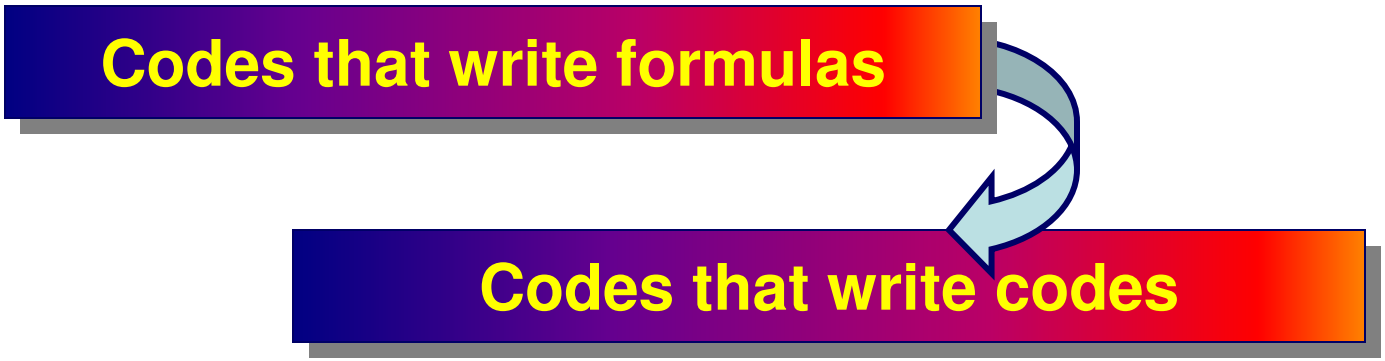
Need total about 300 MB (+extra 150MB file)

Extra index *r* gives at least a factor (35×13) : over 130GB!

The complexity of the equations also increases.

Problem with all-order extensions: TOO MANY TERMS

Solution: automated code generation !



Input: list of formulas to be programmed
Output: final code (need to be put into a main shell)

Features: simple input, essentially just type in a formula!

Monovalent systems: very brief summary of what we calculated with all-order method

Properties

- Energies
- Transition matrix elements (E1, E2, E3, M1)
- Static and dynamic polarizabilities & applications
  - Dipole (scalar and tensor)
  - Quadrupole, Octupole
  - Light shifts
  - Black-body radiation shifts
  - Magic wavelengths
- Hyperfine constants
- C_3 and C_6 coefficients
- Parity-nonconserving amplitudes (derived weak charge and anapole moment)
- EDM enhancement factors
- Isotope shifts (field shift and one-body part of specific mass shift)
- Atomic quadrupole moments
- Nuclear magnetic moment (Fr), from hyperfine data

Systems

Li, Na, Mg II, Al III, Si IV, P V, S VI, K, Ca II, In, In-like ions, Ga, Ga-like ions, Rb, Cs, Ba II, Tl, Fr, Th IV, U V, other Fr-like ions, Ra II

GOALS OF THE OUR PRESENT PROJECT:

1. CALCULATE PROPERTIES OF DIVALENT AND TRIVALENT ATOMS WITH PRECISION COMPARABLE TO ALKALI-METAL ATOMS

2. EXTEND THIS APPROACH TO MORE COMPLICATED SYSTEMS

M. S. Safronova, M. G. Kozlov, S. G. Porsev

Summary of Theory Methods for PNC Calculations

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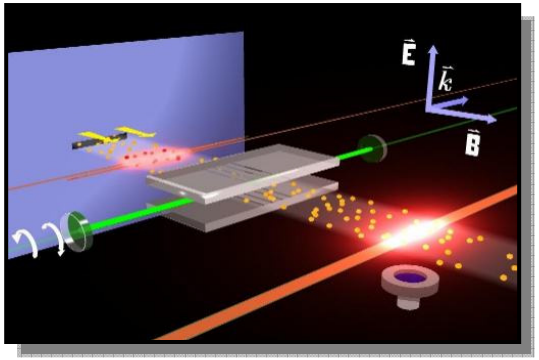
- Configuration interaction + second-order MBPT
- Configuration interaction + coupled-cluster method*

*under development

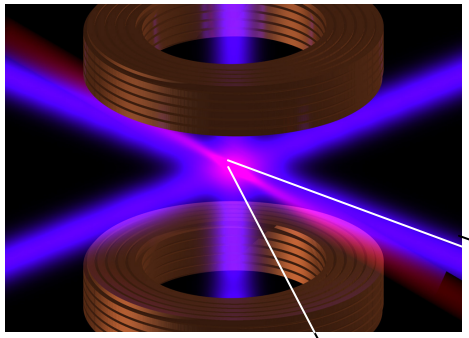
MOTIVATION:
STUDY OF GROUP II – TYPE SYSTEMS

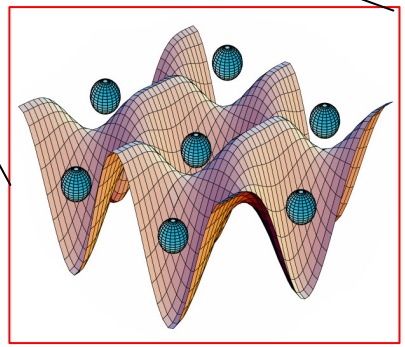
Mg
Ca
Sr
Ba
Ra

Zn
Cd
Hg
Yb



- Study of parity violation
- Search for EDM
- Atomic clocks
- Degenerate quantum gases, alkali-group II mixtures
- Quantum information
- Variation of fundamental constants





Divalent ions: Al^+, In^+, etc.

Configuration Interaction Method

$$\Psi = \sum_i c_i \Phi_i \leftarrow$$ Single-electron valence basis states

$$\left(H^{eff} - E\right)\Psi = 0$$

Example: two particle system:

$$\frac{1}{\left|\mathbf{r}_1 - \mathbf{r}_2\right|}$$

$$H^{eff} = \underbrace{h_1(r_1) + h_1(r_2)}_{\substack{one-body \\ part}} + \underbrace{h_2(r_1, r_2)}_{\substack{two-body \\ part}}$$

Configuration Interaction + Many-Body Perturbation Theory

CI works for systems with many valence electrons but can not accurately account for core-valence and core-core correlations.

MBPT can not accurately describe valence-valence correlation for large systems but accounts well for core-core and core-valence correlations.

Therefore, two methods are combined to acquire benefits from both approaches.

CONFIGURATION INTERACTION METHOD + MBPT

H_{eff} is modified using perturbation theory expressions

$$h_1 \to h_1 + \Sigma_1$$
$$h_2 \to h_2 + \Sigma_2$$

$$\Rightarrow \left(H^{eff} - E\right)\Psi = 0$$

Σ_1, Σ_2 are obtained using perturbation theory

V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov , Phys. Rev. A **54**, 3948 (1996)
V. A. Dzuba and W. R. Johnson , Phys. Rev. A **57**, 2459 (1998)
V. A. Dzuba, V. V. Flambaum, and J. S. Ginges , Phys. Rev. A **61**, 062509 (2000)
S. G. Porsev, M. G. Kozlov, Yu. G. Rakhlina, and A. Derevianko, Phys. Rev. A **64**, 012508 (2001)
M. G. Kozlov, S. G. Porsev, and W. R. Johnson, Phys. Rev. A **64**, 052107 (2001)
I. M. Savukov and W. R. Johnson, Phys. Rev. A 65, 042503 (2002)
Sergey G. Porsev, Andrei Derevianko, and E. N. Fortson, Phys. Rev. A **69**, 021403 (2004)
V. A. Dzuba and J. S. Ginges, Phys. Rev. A **73**, 032503 (2006)
V. A. Dzuba and V. V. Flambaum , Phys. Rev. A **75**, 052504 (2007)

CONFIGURATION INTERACTION METHOD + MBPT

H_{eff} is modified using perturbation theory expressions

$$h_1 \rightarrow h_1 + \Sigma_1$$
$$h_2 \rightarrow h_2 + \Sigma_2$$

$$\Rightarrow \left(H^{eff} - E\right)\Psi = 0$$

Σ_1, Σ_2 are obtained using perturbation theory

Problem: accuracy deteriorates for heavier systems owing to larger correlation corrections

CONFIGURATION INTERACTION + COUPLED-CLUSTER METHOD

H_{eff} is modified using all-order excitation coefficients

$$\left(\Sigma_1\right)_{mn} = \left(\tilde{\varepsilon}_n - \varepsilon_m\right)\rho_{mn}$$

$$\left(\Sigma_2\right)^L_{mnkl} = \left(\tilde{\varepsilon}_k + \tilde{\varepsilon}_l - \varepsilon_m - \varepsilon_n\right)\rho^L_{mnkl}$$

Advantages: most complete treatment of the correlations and applicable for many-valence electron systems

CI + ALL-ORDER RESULTS

Two-electron binding energies, differences with experiment

Atom	CI	CI + MBPT	CI + All-order
Mg	1.9%	0.11%	0.03%
Ca	4.1%	0.7%	0.3%
Zn	8.0%	0.7%	0.4 %
Sr	5.2%	1.0%	0.4%
Cd	9.6%	1.4%	0.2%
Ba	6.4%	1.9%	0.6%
Hg	11.8%	2.5%	0.5%
Ra	7.3%	2.3%	0.67%

Development of a configuration-interaction plus all-order method for atomic calculations, M.S. Safronova, M. G. Kozlov, W.R. Johnson, Dansha Jiang, Phys. Rev. A 80, 012516 (2009).

3. Applications to Atomic Clocks – BBR Shifts

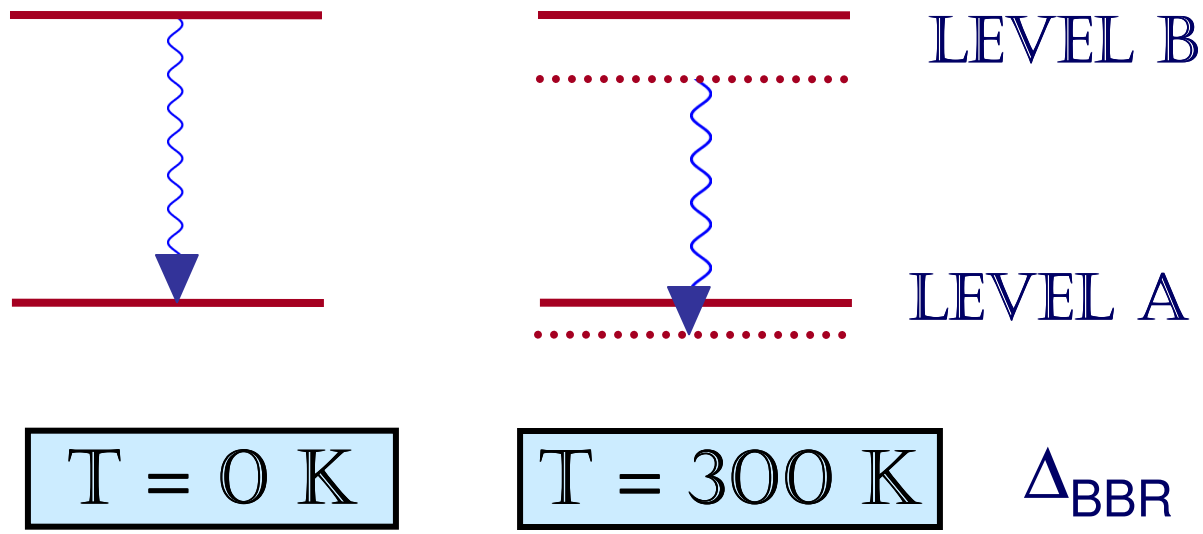
Precision Calculation of Blackbody Radiation Shifts for Optical Frequency Metrology

M.S. Safronova, M. G. Kozlov and C. W. Clark

Physical Review Letters, 107, 143006 (2011) .

BLACKBODY RADIATION SHIFTS

CLOCK TRANSITION



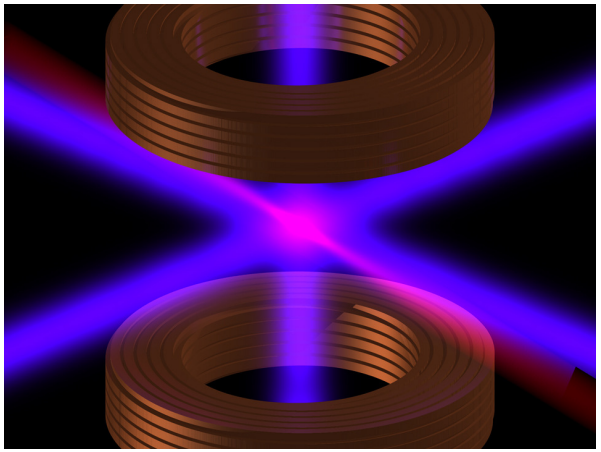
Transition frequency should be corrected to account for the effect of the black body radiation at T=300K.

ATOMIC CLOCKS
BLACK-BODY RADIATION (BBR) SHIFT

Motivation:

BBR shift gives large contribution into uncertainty budget for some of the atomic clock schemes.

Accurate calculations (or measurements) are needed to achieve ultimate precision goals at room temperature.



Summary of the fractional uncertainties $\Delta\nu/\nu_0$ due to BBR shift and the fractional error in the absolute transition frequency induced by the BBR shift uncertainty at T = 300 K in various frequency standards

Atom	Clock transition	$\Delta\nu/\nu_0$	Uncertainty	Reference
Rb	5s (F=2 - F=1)	-1.25×10^{-14}	4×10^{-17}	Safronova et al. 2010
Cs	6s (F=4 - F=3)	-1.7×10^{-14}	3×10^{-17}	Simon et al. 1998
Ca^+	$4s - 3d_{5/2}$	9.2×10^{-16}	1×10^{-17}	Safronova et al. 2011
Sr^+	$5s - 4d_{5/2}$	5.6×10^{-16}	2×10^{-17}	Jiang et al. 2009
Yb^+	$6s - 5d\ ^2D_{3/2}$	-5.3×10^{-16}	1×10^{-16}	Tamm et al. 2007
Yb^+	$6s - 4f^{13}\ 6s^2\ ^2F_{7/2}$	-5.7×10^{-17}	1×10^{-17}	Hosaka et al 2009
Mg	$3s^2\ ^1S_0 - 3s3p\ ^3P_0$	-3.9×10^{-16}	1×10^{-17}	Porsev et al. 2006
Al^+	$3s^2\ ^1S_0 - 3s3p\ ^3P_0$	-7×10^{-18}	3×10^{-18}	Rosenband et al. 2006
Sr	$5s^2\ ^1S_0 - 5s5p\ ^3P_0$	-5.5×10^{-15}	7×10^{-17}	Porsev et al. 2006
Yb	$6s^2\ ^1S_0 - 6s6p\ ^3P_0$	-2.6×10^{-15}	3×10^{-16}	Porsev et al. 2006
Hg	$6s^2\ ^1S_0 - 6s6p\ ^3P_0$	-1.6×10^{-16}		Hachisu et al. 2008

TOPICAL REVIEW: Theory and applications of atomic and ionic polarizabilities,
J. Mitroy, M.S. Safronova, and C.W. Clark, J. Phys. B: At. Mol. Opt. Phys. 43 (2010) 202001

M. S. Safronova *et al.*, IEEE - TUFFC 57, 94 (2010)

BBR SHIFT OF A LEVEL

- The temperature-dependent electric field created by the blackbody radiation is described by (in a.u.) :

$$E^2(\omega) = \frac{8\alpha}{\pi} \frac{\omega^3 d\omega}{\exp(\omega / kT) - 1}$$

- Frequency shift caused by this electric field is:

$$\Delta\nu_{\mathrm{BBR}} = -A \times \int \alpha(\omega) E^2(\omega)\, d\omega$$

Dynamic polarizability

BBR SHIFT AND POLARIZABILITY

BBR shift of atomic level can be expressed in terms of a **scalar static polarizability** to a good approximation [1]:

$$\Delta\nu_{\mathrm{BBR}} = -\frac{1}{2}\alpha_0(0)(831.9V/m)^2\left(\frac{T(K)}{300}\right)^4(1+\eta)$$

Dynamic correction

Dynamic correction is generally small.

Multipolar corrections (M1 and E2) are suppressed by α^2 [1].

VECTOR & TENSOR POLARIZABILITY AVERAGE OUT DUE TO THE ISOTROPIC NATURE OF FIELD.

[1] Sergey Porsev and Andrei Derevianko, Physical Review A 74, 020502R (2006)

Al^+ energy levels, differences with experiment

Level		CI	CI+MBPT	CI+All
$3s^2$	$^1S_0$	1.2%	0.043%	0.006%
$3p^2$	$^1D_2$	2.3%	0.07%	-0.022%
3s4s	$^3S_1$	1.4%	0.07%	0.015%
$3p^2$	$^3P_0$	1.6%	0.04%	0.008%
$3p^2$	$^3P_1$	1.6%	0.03%	0.004%
$3p^2$	$^3P_2$	1.6%	0.02%	-0.004%
3s4s	$^1S_0$	1.4%	0.05%	0.003%
3s3p	$^3P_0$	3.1%	0.15%	0.007%
3s3p	$^3P_1$	3.1%	0.14%	0.008%
3s3p	$^3P_2$	3.1%	0.12%	-0.017%
3s3p	$^1P_1$	0.4%	-0.17%	-0.14%

Al^+ POLARIZABILITIES (A.U.)

	CI	CI+MBPT	CI + All-order
α ($3s^2\ ^1S_0$)	24.405	24.030	24.408
α ($3s3p\ ^3P_0$)	24.874	24.523	24.543
$\Delta\alpha$($^3P_0$ - $^1S_0$)	0.469	0.493	0.495

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Accuracy of $\Delta\alpha$ ($^3P_0$ - $^1S_0$) ?

Difference (CI+MBPT → CI + all-order) = 0.4%
Difference (CI → CI + all-order) = 2.6 %
Other uncertainties: 1.4% (Breit) and 2% (core)

Estimate: 10%

Sr POLARIZABILITIES (a.u.)

Sr	CI +MBPT	CI+all-order	Recomm.*
$5s^2\ ^1S_0$	195.6	198.0	197.2(2)
$5s5p\ ^3P_0$	483.6	459.4	458.3(3.6)

*From expt. matrix elements, S. G. Porsev and A. Derevianko, PRA 74, 020502R (2006).

Summary of the fractional uncertainties $\Delta\nu/\nu_0$ due to BBR shift and the fractional error in the absolute transition frequency induced by the BBR shift uncertainty at T = 300 K in various frequency standards

Atom	Clock transition	$\Delta\nu/\nu_0$	Uncertainty	Reference
Rb	5s (F=2 - F=1)	-1.25×10^{-14}	4×10^{-17}	Safronova et al. 2010
Cs	6s (F=4 - F=3)	-1.7×10^{-14}	3×10^{-17}	Simon et al. 1998
Ca^+	$4s - 3d_{5/2}$	9.2×10^{-16}	1×10^{-17}	Safronova et. Al, 2011
Sr^+	$5s - 4d_{5/2}$	5.6×10^{-16}	2×10^{-17}	Jiang et al. 2009
Yb^+	$6s - 5d\ ^2D_{3/2}$	-5.3×10^{-16}	1×10^{-16}	Tamm et al. 2007
Yb^+	$6s - 4f^{13}\ 6s^2\ ^2F_{7/2}$	-5.7×10^{-17}	1×10^{-17}	Hosaka et al 2009
Mg	$3s^2\ ^1S_0 - 3s3p\ ^3P_0$	-3.9×10^{-16}	1×10^{-17}	Porsev et al. 2006
B^+	$2s^2\ ^1S_0 - 2s2p\ ^3P_0$	1.42×10^{-17}	1×10^{-18}	This work
Al^+	$3s^2\ ^1S_0 - 3s3p\ ^3P_0$	-3.8×10^{-18}	4×10^{-19}	This work
In^+	$5s^2\ ^1S_0 - 5s5p\ ^3P_0$	-1.36×10^{-17}	1×10^{-18}	This work
Sr	$5s^2\ ^1S_0 - 5s5p\ ^3P_0$	-5.5×10^{-15}	7×10^{-17}	Porsev et al. 2006
Yb	$6s^2\ ^1S_0 - 6s6p\ ^3P_0$	-2.6×10^{-15}	3×10^{-16}	Porsev et al. 2006
Hg	$6s^2\ ^1S_0 - 6s6p\ ^3P_0$	-1.6×10^{-16}		Hachisu et al. 2008

SUMMARY: BBR SHIFTS

We have performed the calculations of the BBR shifts in B^+, Al^+, and In^+ that allowed to reduce the ultimate uncertainties due to this effect at room temperature to 10^{-18} level for B^+ and In^+ and to 4×10^{-19} for Al^+.

These uncertainties approach recent estimates of the feasible precision of currently proposed optical atomic clocks.

Future: addition of more all-order correlation corrections for further improvement of accuracy, BBR in Yb, Hg, and Sr.

4. TL EDM ENHANCEMENT FACTOR CONTROVERSY

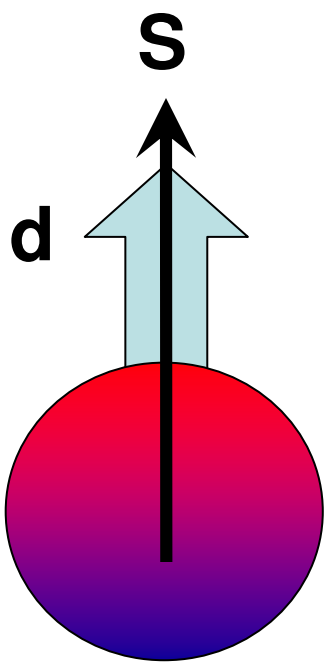
Electric Dipole Moment Enhancement Factor of Thallium

S. G. Porsev, M. S. Safronova, and M. G. Kozlov,

Phys. Rev. Lett. 108, 173001 (2012)

Permanent electric-dipole moment (EDM)

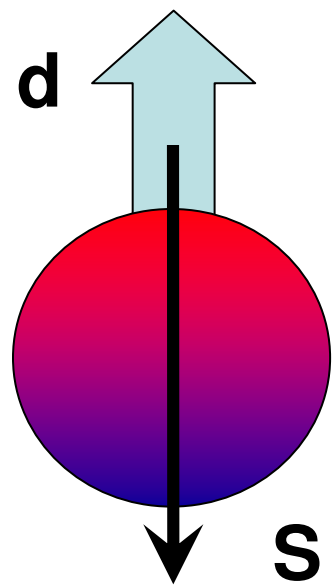
Time-reversal invariance must be violated for an elementary particle or atom to possess a permanent EDM.



$$t \rightarrow -t$$

$$\vec{\mathbf{S}} \rightarrow -\vec{\mathbf{S}}$$

$$\vec{\mathbf{d}} \rightarrow \vec{\mathbf{d}}$$

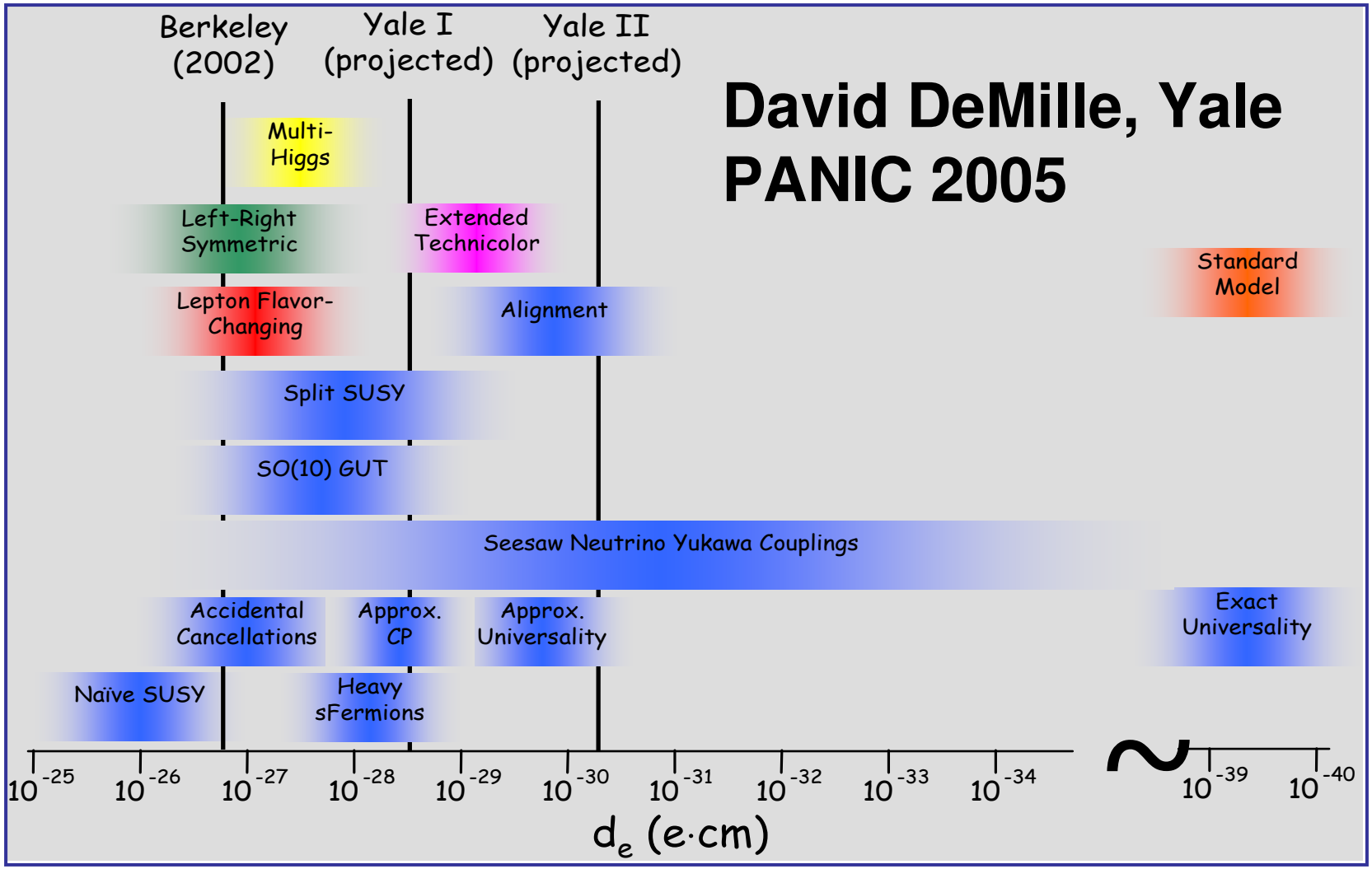


$$\vec{\mathbf{d}} = d\,\frac{\vec{\mathbf{S}}}{S}$$

$$d = 0$$

EDM and new physics

Many theories beyond the Standard Model predict electron EDM within or just beyond the present experimental capabilities.



Atomic calculations and search for EDM

EDM effects are enhanced in some heavy atoms and molecules.

Limits on the electron EDM

Tl atom: $|d_e| < 1.6 \times 10^{-27}$ e cm

Regan et al., Phys. Rev. Lett.88, 071805 (2002)

YbF molecule: $|d_e| < 1.05 \times 10^{-27}$ e cm

Hudson et al., Nature 473, 493 (2011)

Both results crucially depend on the calculated values of the effective electric field on the valence electron. In the case of Tl this effective field is proportional to the applied field E_0,
$E = K E_0$ and $d(^{205}\mathrm{Tl}) = K d_e$, ***K = - 585***

Tl EDM enhancement factor controversy

Z. W. Liu and H. P. Kelly, PRA 45, R4210 (1992).

K = - 585 (30-60)

V.A. Dzuba and V. V. Flambaum, PRA 80, 062509 (2009)

K = - 582 (20)

Tl EDM enhancement factor controversy

Z. W. Liu and H. P. Kelly, PRA 45, R4210 (1992).

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K = - 582 (20)

H. S. Nataraj, B. K. Sahoo, B. P. Das, and D. Mukherjee, PRL 106, 200403 (2011)

K = - 466 (10)

Tl EDM enhancement factor

[1] V.A. Dzuba and V. V. Flambaum, PRA 80, 062509 (2009)
[2] H. S. Nataraj, B. K. Sahoo, B. P. Das, and D. Mukherjee, PRL 106, 200403 (2011)

	Ref. [1]	Ref. [2]	Difference
Result	**- 582(20)**	**- 466(10)**	**25% or 5σ**
Method	CI+MBPT	CCSD(T)	
Potential	V^{N-3} fully three particle treatment $5d^{10}$ core	V^{N-1} treats Tl as Cs $5d^{10}6s^2$ core	
Correlations Core	S - all-order D – second-order	SD all-order	
Valence	all-order (via CI)	all-order	
Numerical Issues	CI basis restriction MBPT part restriction	Basis 38s, 34p, 34d, 30f, 20g CCSD basis 14s, 13p, 13d, 9f, 8g	
Other issues		Drastic dif. with CCSD of Liu and Kelly	

Present work: Calculation # 1

1a. We have repeated the CI+MBPT calculation of Dzuba and Flambaum in V^{N-3} potential and ensured that we agree with their value at the same level of approximation (-578 vs. -582).

1b. We have calculated a number of corrections that were omitted in 2009, including structure radiation, core-Brueckner, two-particle, selected three-particle, and normalization corrections.

We found that some of these corrections are large, 5 - 7% percent, but partially canceling, causing lower accuracy of V^{N-3} CI+MBPT results than was previously expected.

Present work: Calculation # 2

2. We have carried out the **CI + all-order** calculation in the same V^{N-3} potential – all previous corrections included.

This calculation allowed us to evaluate the effect of higher-order core-core and core-valence corrections to the EDM (omitted in CI+MBPT).

We found that the effect of these corrections to the enhancement factor is small, 0.7%.

Result in V^{N-3}: K = - 538(46) instead of K = - 582(20) in [1]

[1] V.A. Dzuba and V. V. Flambaum, PRA 80, 062509 (2009)

Present work: Calculation # 3

3. We have carried out the **CI + MBPT** calculation in the V^{N-1} potential used in [2]. We still treat all three valence electrons using CI. Therefore, we can accurately treat the contributions of the $6s6p^2$ states to K on the same footing as the $6s^2ns$ states in contrast with the work of Nataraj et al., (2011).

Final result in V^{N-1}: K = - 573(20)

Uncertainty estimate:

(a) Accuracy of relevant hyperfine constants and E1 matrix elements is 3% or better.

(b) CI value is K = - 594. All other corrections contribute 3.7%.

Present work: Calculation # 4

4. In an attempt to compare with coupled-cluster calculations of [2], we carried out full relativistic coupled-cluster calculations in V^{N-1} potential.

Contribution to K	CI+MBPT	CC (present)	CC [2]
$6s^2 7s\ ^2S_{1/2}$	**-216.6**	**-212.2**	**-188**
$6s^2 8s\ ^2S_{1/2}$	**-22.4**	**-22.8**	
$6s6p^2\ ^4P_{1/2}$	-74.6		
$6s6p^2\ ^2P_{1/2}$	-179.2		
$6s6p^2\ ^4D_{1/2}$?	1.3		
Other	-81.1		
Total (present work)	-572.5		

[2] H. S. Nataraj, B. K. Sahoo, B. P. Das, and D. Mukherjee, PRL 106, 200403 (2011)

Present work: Calculation # 4b

4b. Comparison with Ref. [2]: basis set issues.

Basis in [2]: **38s, 34p, 34d, 30f, 20g**

Basis used in coupled-cluster calculation of [2]: **14s, 13p, 13d, 9f**

We have conducted another coupled-cluster calculations with a truncated basis that we have constructed using parameters of [2].

The truncation of the basis set to the size of the one used in Ref. [2] produced very large reduction (by 18%) in the value of the $6p_{1/2}$ - 7s EDM matrix element.

<u>Other corrections:</u>

Breit interaction effect on the EDM: negligible (0.36%).

Summary: Tl EDM enhancement factor

Z. W. Liu and H. P. Kelly, PRA 45, R4210 (1992).

K = - 585 (30-60)

V.A. Dzuba and V. V. Flambaum, PRA 80, 062509 (2009)

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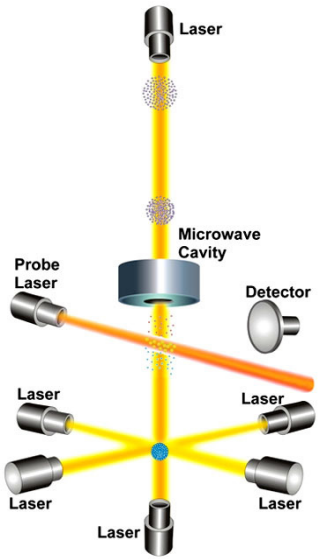
H. S. Nataraj, B. K. Sahoo, B. P. Das, and D. Mukherjee, PRL 106, 200403 (2011)

K = - 466 (10)

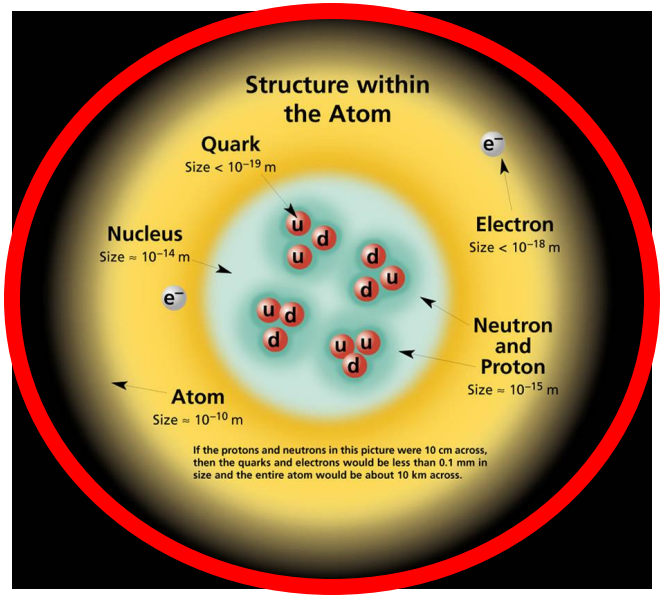
S. G. Porsev, M. S. Safronova, and M. G. Kozlov, arXiv:1201.5615, Phys. Rev. Lett, in press, April 2012

K = - 573 (20) - several calculations carried out

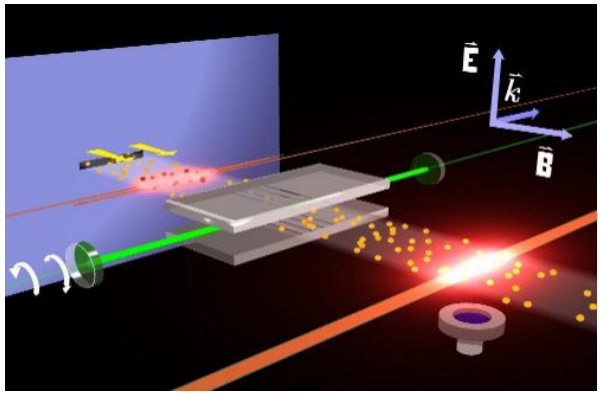
CONCLUSION

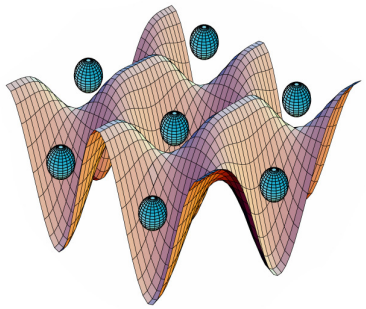


Atomic Clocks

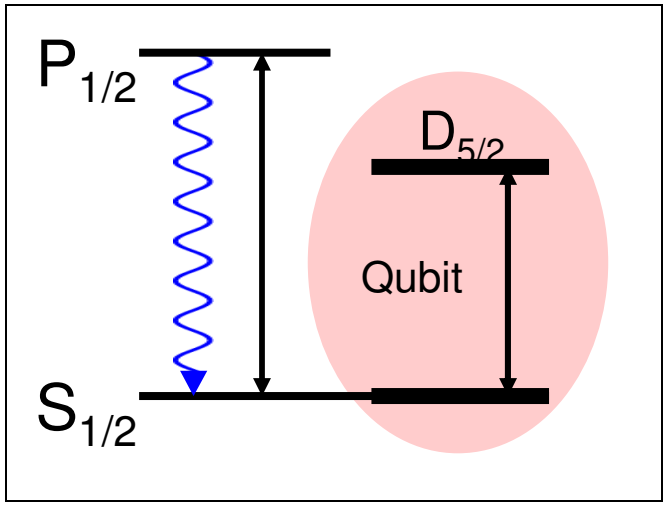


Parity Violation





Future:
New Systems
New Methods,
New Problems



Quantum information

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