

University of Virginia Colloquium

ATOMIC CALCULATIONS FOR TESTS OF FUNDAMENTAL PHYSICS

MARIANNA SAFRONOVA



NIST

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



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OUTLINE

- **Atomic physics tests of fundamental physics**
 - Parity violation
 - Search for permanent electric-dipole moment (EDM)
 - Variation of fundamental constants and atomic clocks
- **Atomic parity violation**
 - Theory: How to calculate APV amplitude?
 - Analysis of Cs experiment and implications for search for physics beyond the Standard Model
 - Nuclear spin-dependent APV effects and weak hadronic interactions

TRANSFORMATIONS AND SYMMETRIES

Translation	→	Momentum conservation
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Translation in time	→	Energy conservation
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Rotation	→	Conservation of angular momentum
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[C] Charge conjugation	→	C-invariance
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[P] Spatial inversion	→	Parity conservation (P-invariance)
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[T] Time reversal	→	T-invariance
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[CP]

[CPT]

TRANSFORMATIONS AND SYMMETRIES

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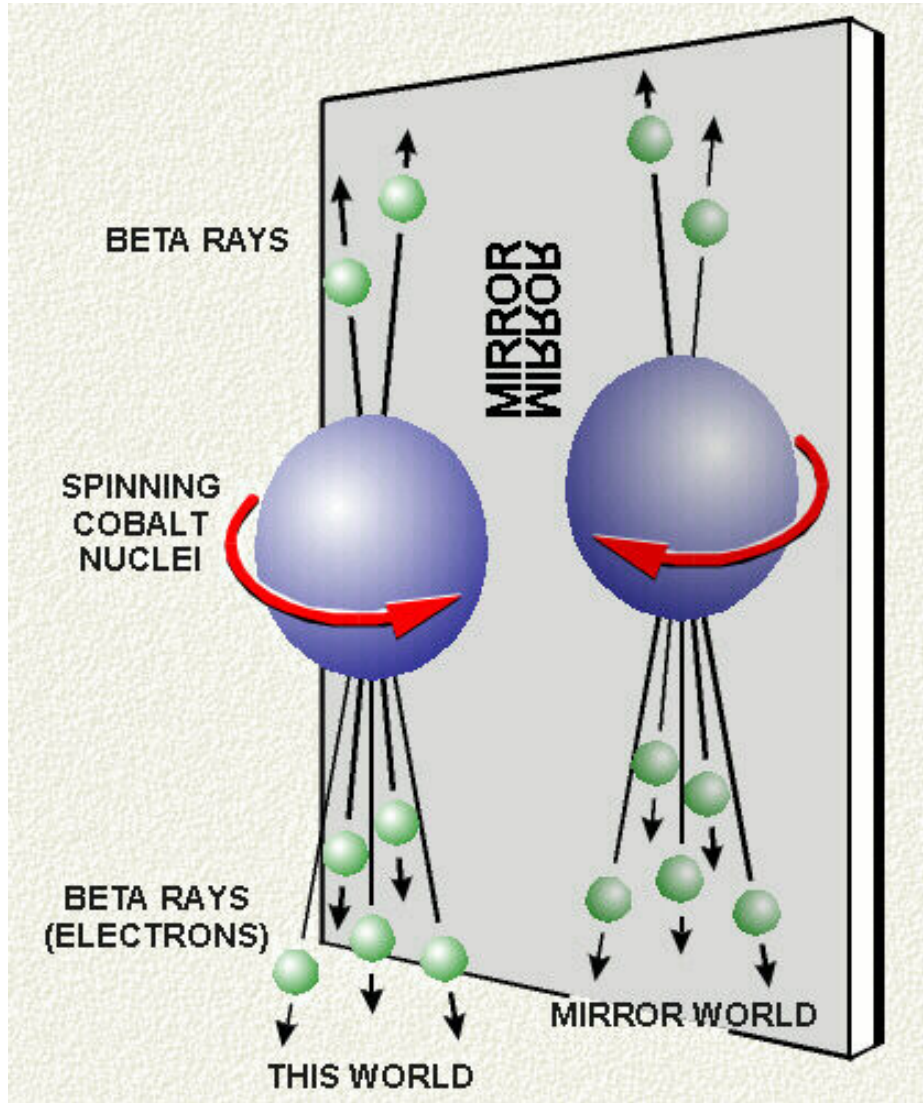
[T] Time reversal → T-invariance

[CP]

[CPT]

Parity Violation

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

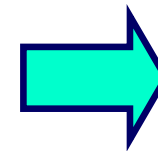


Parity-transformed world:

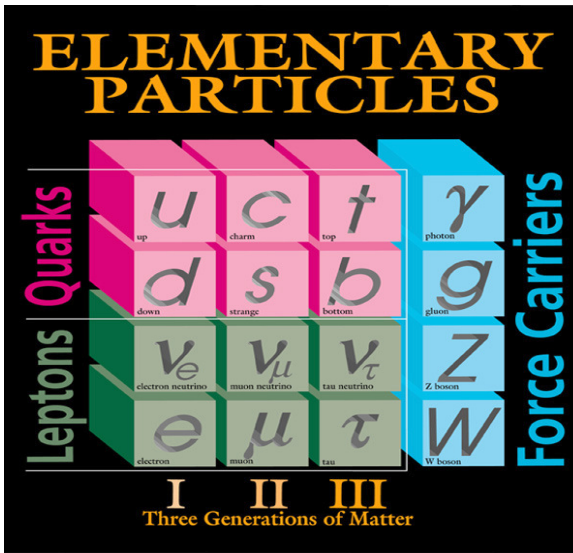
Turn the mirror image upside down.

The parity-transformed world is not identical with the real world.

Weak		
(Electron)		
Flavor		
Quarks, Leptons		
W^+	W^-	Z^0
0.8		
10^{-4}		
10^{-7}		



Parity is not conserved.



STANDARD MODEL

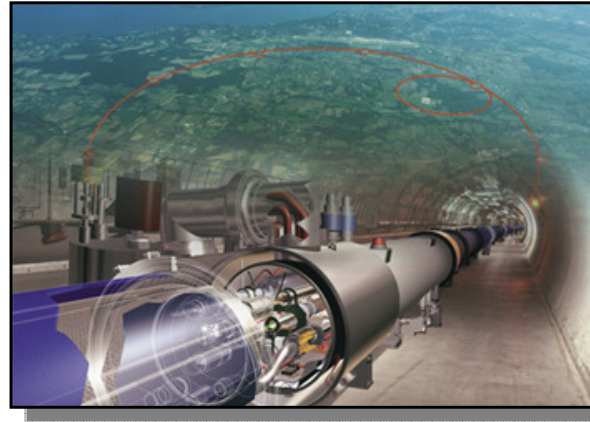
PROPERTIES OF THE INTERACTIONS

Property \ Interaction	Gravitational	Weak (Electroweak)	Electromagnetic	Strong	
				Fundamental	Residual
Acts on:	Mass – Energy	Flavor	Electric Charge	Color Charge	See Residual Strong Interaction Note
Particles experiencing:	All	Quarks, Leptons	Electrically charged	Quarks, Gluons	Hadrons
Particles mediating:	Graviton (not yet observed)	W^+ W^- Z^0	γ	Gluons	Mesons
Strength relative to electromag for two u quarks at:	10^{-18} m	0.8	1	25	Not applicable to quarks
	3×10^{-17} m	10^{-4}	1	60	
	for two protons in nucleus	10^{-36}	1	Not applicable to hadrons	20

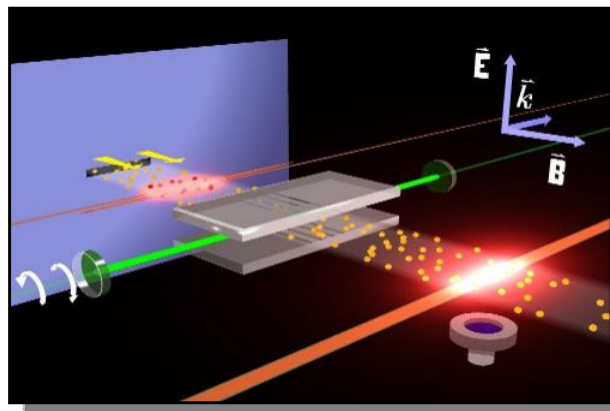
Atomic Parity Violation

High energies

Instead of search for new processes or particles directly



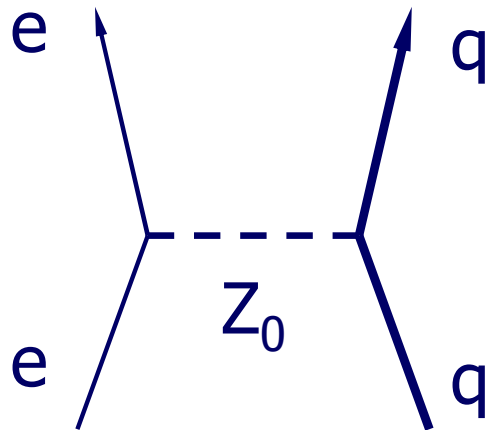
Determine **weak charge** Q_W from atomic parity violation studies and compare the result with Standard Model prediction



Low energies

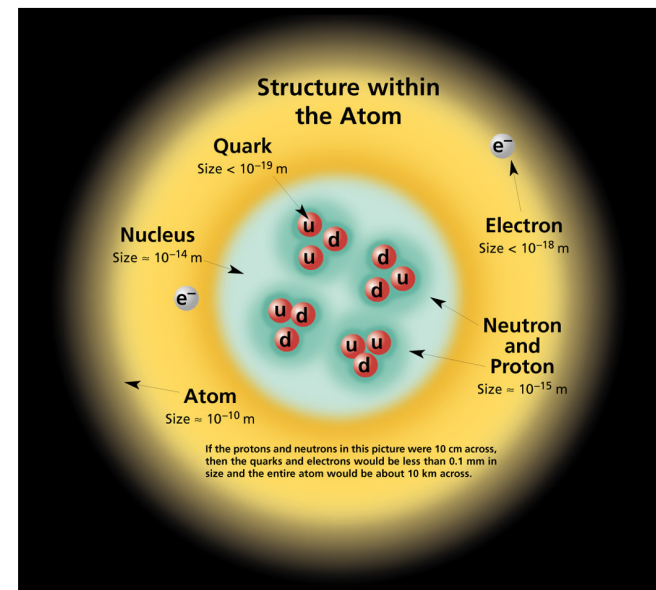
PARITY VIOLATION IN ATOMS

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



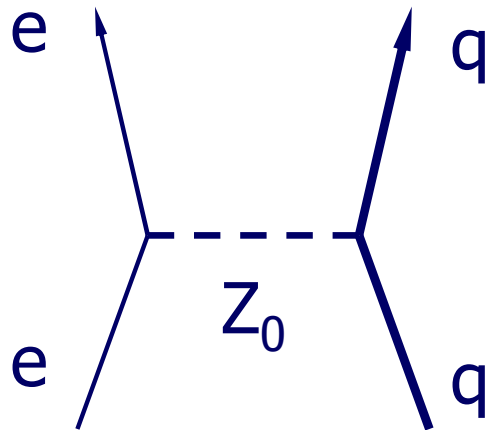
Weak Charge Q_W

Quantifying the strength of the electroweak coupling between atomic electrons and quarks of the nucleus.



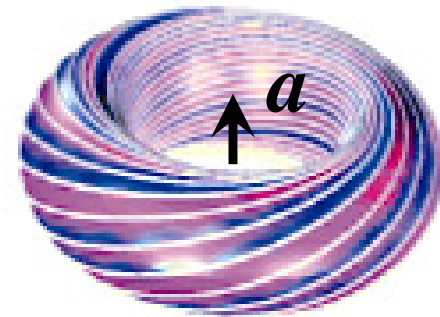
Two sides of the atomic parity violation

NUCLEAR
SPIN-INDEPENDENT
PNC:
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Weak Charge Q_W

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



**Nuclear anapole
moment**

TRANSFORMATIONS AND SYMMETRIES

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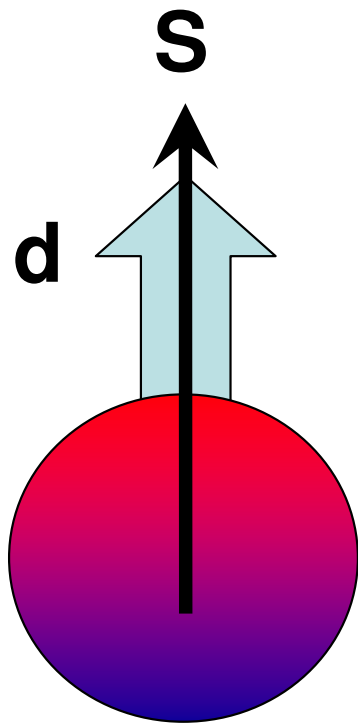
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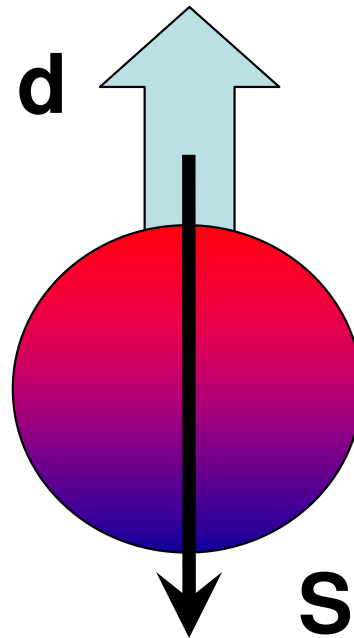
[CPT]

PERMANENT ELECTRIC-DIPOLE MOMENT (EDM)

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



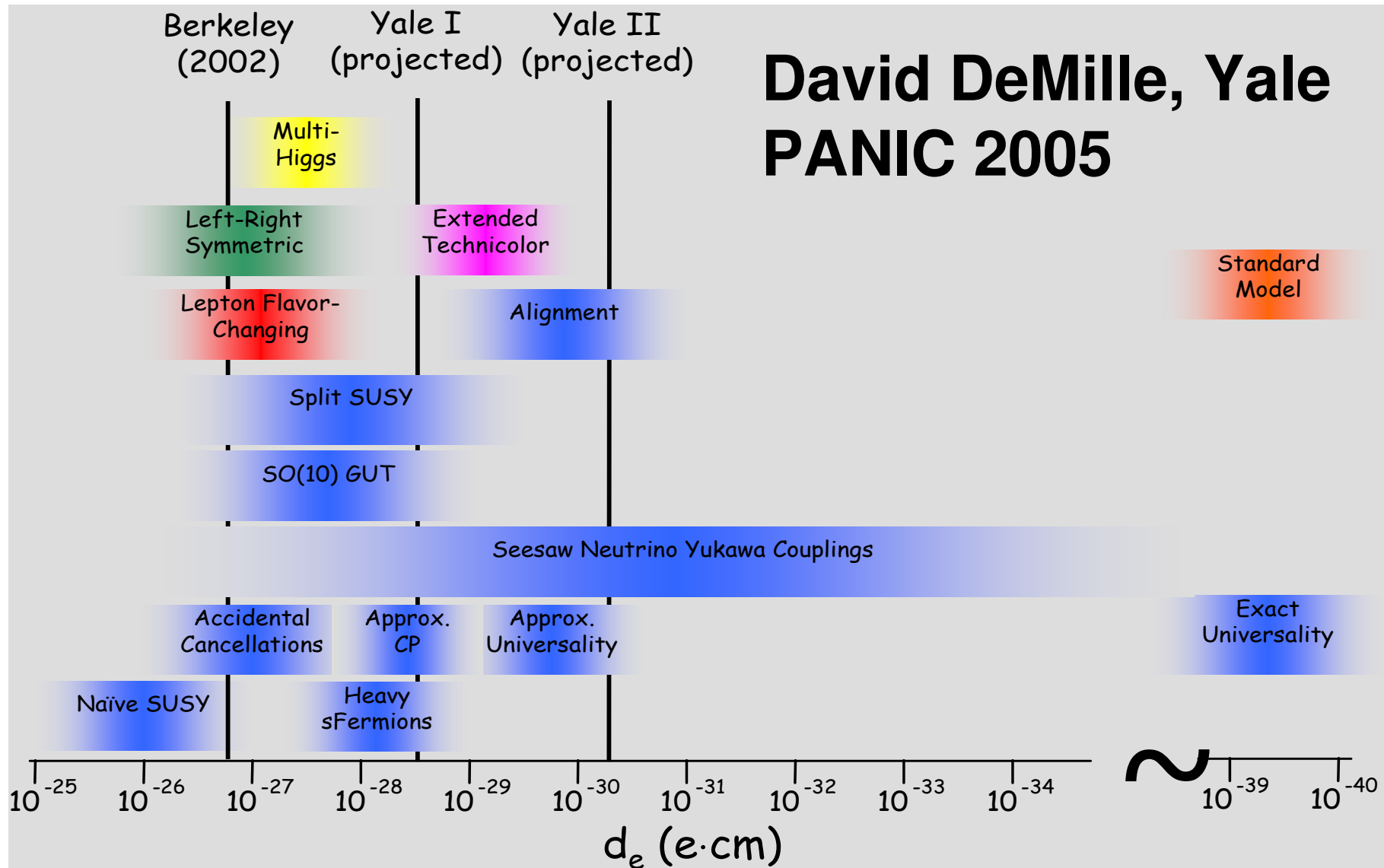
$$\begin{aligned} t &\rightarrow -t \\ \vec{S} &\rightarrow -\vec{S} \\ \vec{d} &\rightarrow \vec{d} \end{aligned}$$



$$\begin{aligned} \vec{d} &= d \frac{\vec{S}}{S} \\ d &= 0 \end{aligned}$$

EDM AND NEW PHYSICS

Many theories beyond the Standard Model predict 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.

Theory is needed to calculate enhancement factors and search for new systems for EDM detection.

Recent new limit on the EDM of ^{199}Hg

$$|d(^{199}\text{Hg})| < 3.1 \times 10^{-29} \text{ e cm}$$

Phys. Rev. Lett.102, 101601 (2009)

ATOMIC CALCULATIONS AND VARIATION OF FUNDAMENTAL CONSTANTS

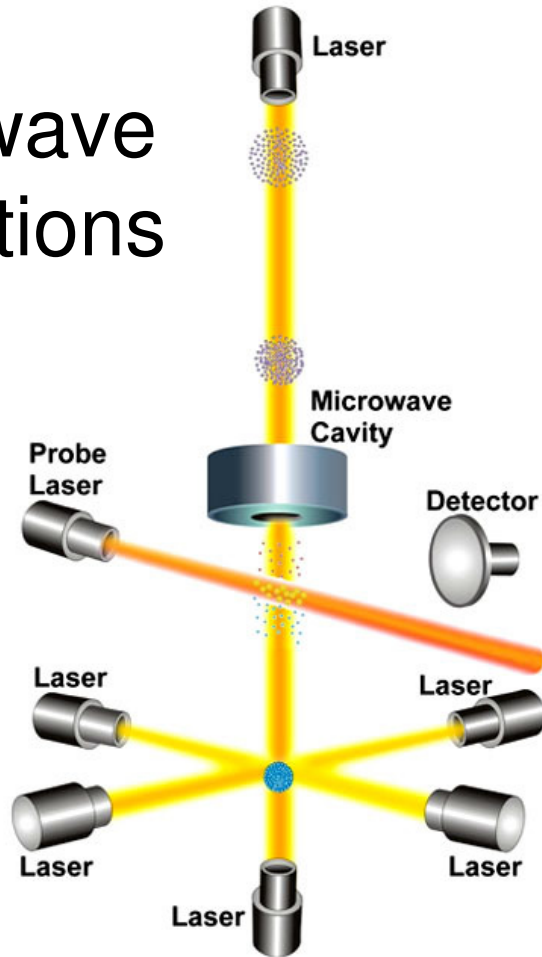
- (1) **Astrophysical constraints** on variation of α :
Study of quasar absorption spectra: **4σ variation!!!**

Atomic calculations: need to know isotope shifts
Changes in isotopic abundances mimic shift of α
- (2) **Laboratory atomic clock experiments:**
compare rates of different clocks over long period of time to study time variation of fundamental constants

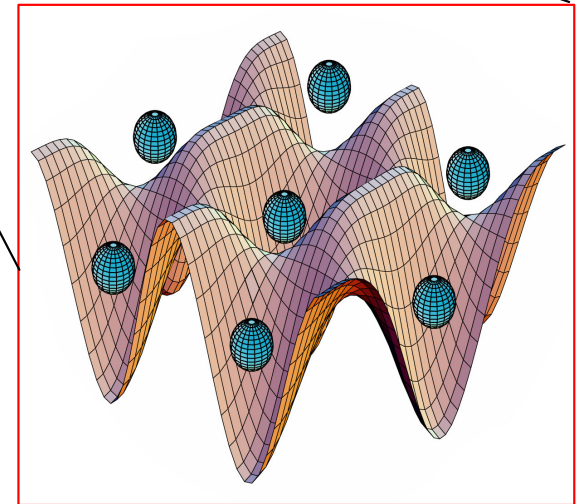
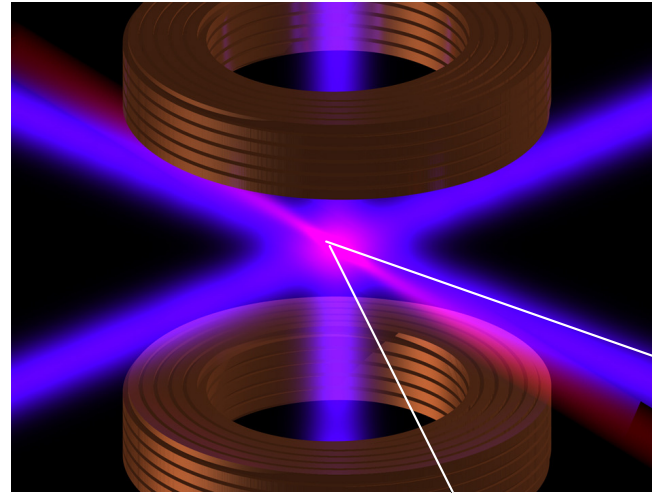
Need: dependence of transition frequency on α and ultra precise clocks!

ATOMIC CLOCKS

Microwave Transitions

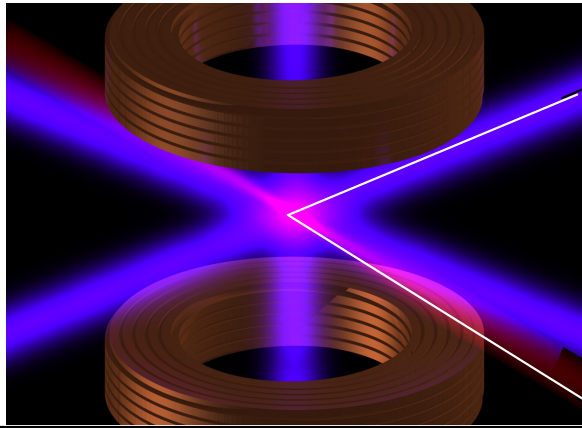


Optical Transitions

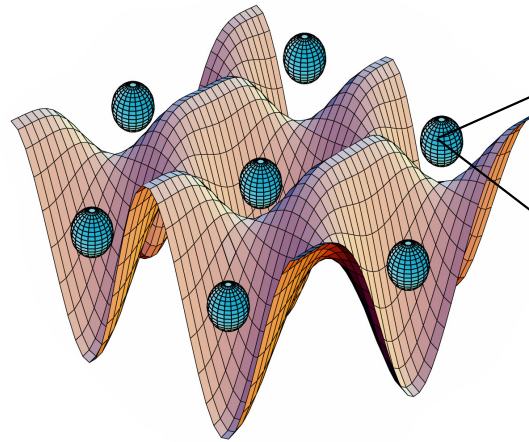


***Blackbody Radiation Shifts and Theoretical Contributions to Atomic Clock Research*, M. S. Safronova, Dansha Jiang, Bindiya Arora, Charles W. Clark, M. G. Kozlov, U. I. Safronova, and W. R. Johnson, in press, Special Issue of IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control (2010).**

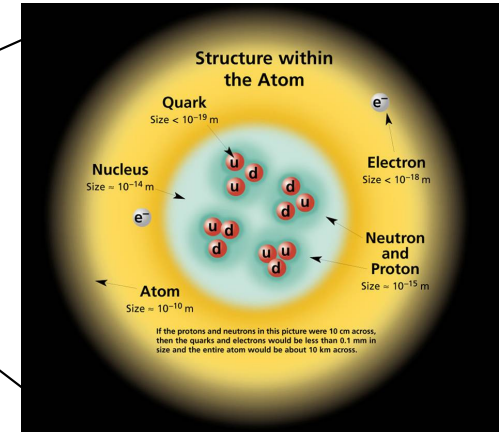
MOTIVATION: NEXT GENERATION ATOMIC CLOCKS



**Next - generation
ultra precise atomic clock**



Atoms trapped by laser light



<http://CPEPweb.org>

The ability to develop more precise optical frequency standards will open ways to improve global positioning system (GPS) measurements and tracking of deep-space probes, perform more accurate measurements of the physical constants and tests of fundamental physics such as searches for gravitational waves, etc.

ATOMIC CALCULATIONS & MORE PRECISE CLOCKS

(1) Prediction of atomic properties required for new clock proposals

New clock proposals require both estimation of the atomic properties for details of the proposals (transition rates, lifetimes, branching ratios, magic wavelength, scattering rates, etc.) and evaluation of the systematic shifts (Zeeman shift, electric quadrupole shift, blackbody radiation shift, ac Stark shifts due to various laser fields, etc.).

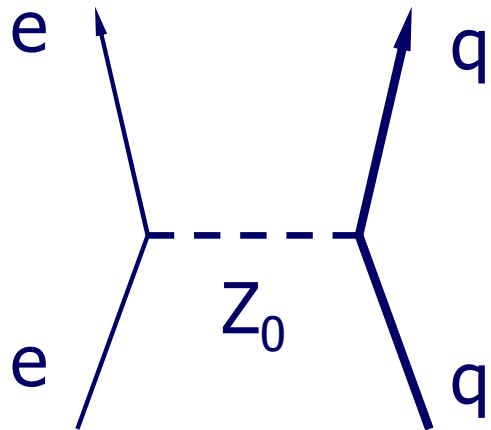
(2) Determination of the quantities contributing to the uncertainty budget of the existing schemes.

In the case of the well-developed proposals, one of the main current uncertainty issues is the blackbody radiation shift.

ATOMIC PARITY VIOLATION

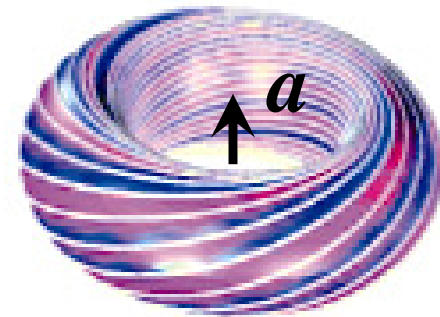
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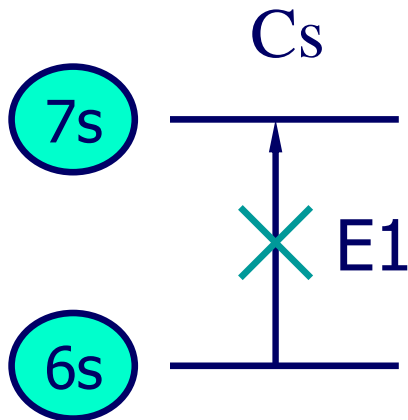
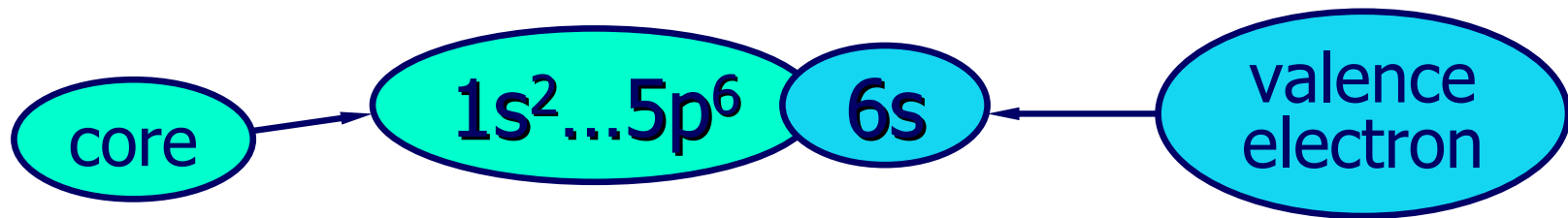
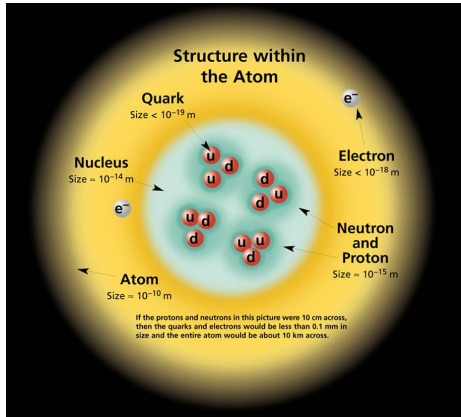


**Nuclear anapole
moment**

Cesium: atom with single (valence) electron outside a closed core.

Cs $Z=55$

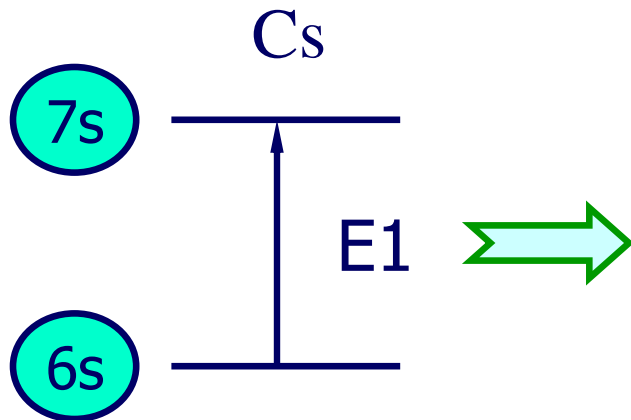
Need heavy atom for atomic PNC



$l=0$ to $l=0$ electric dipole transition is forbidden by parity selection rules

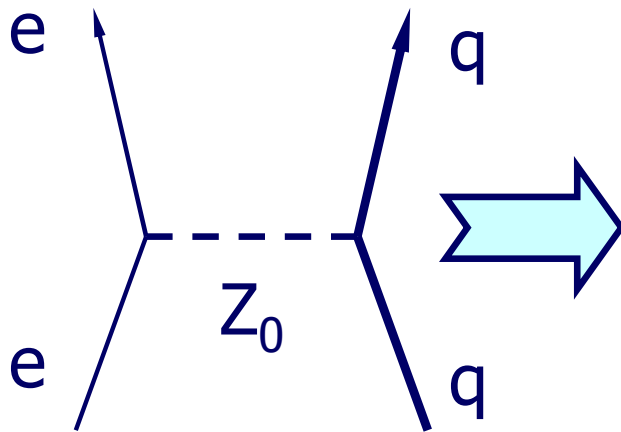
Atomic Parity Violation

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



**Non-zero transition amplitude
PNC amplitude E_{PNC}**

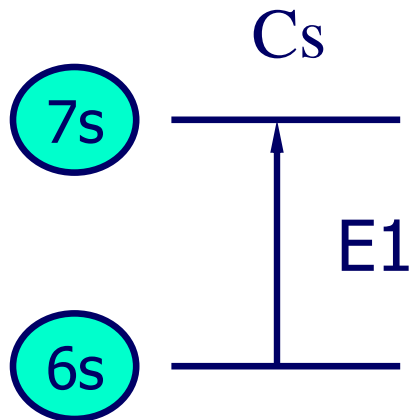
Both 6s and 7s states acquire an
opposite-parity ($np_{1/2}$) admixture



Z_0 exchange: Laporte's rule is violated!

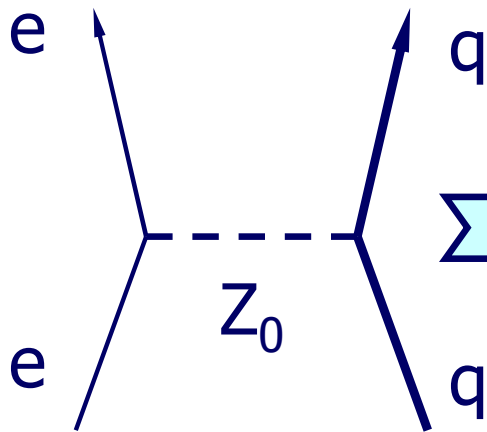
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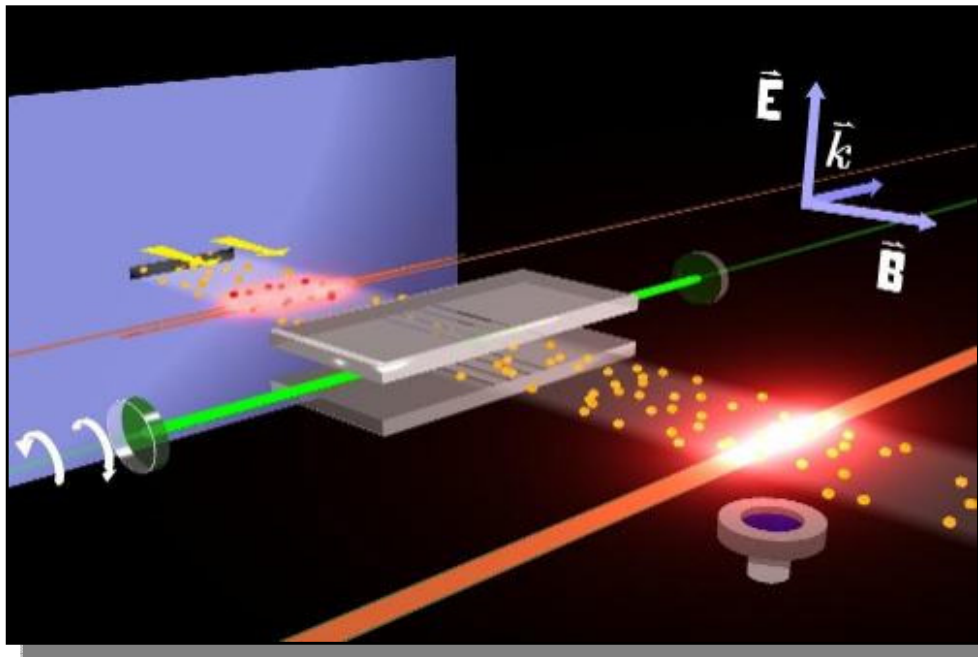


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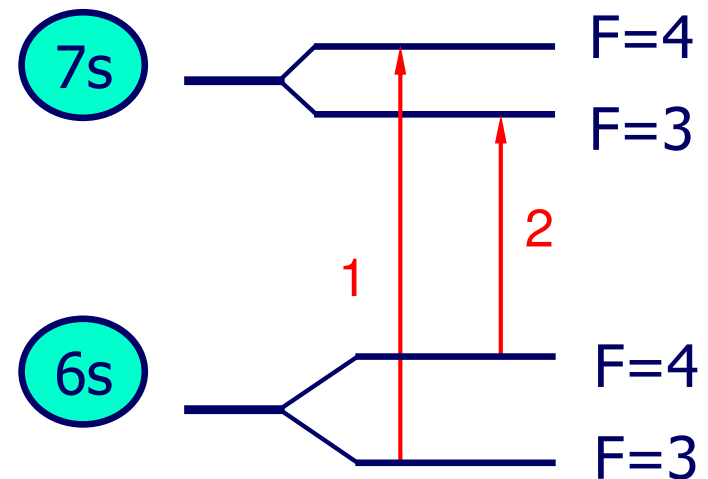
Note: it is really tiny effect !!! $E_{\text{PNC}} \sim 10^{-11}$ atomic units
E1 amplitude for 6s – 6p transition is **4.5** atomic units

The most precise measurement of PNC amplitude (cesium)

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



0.35% accuracy

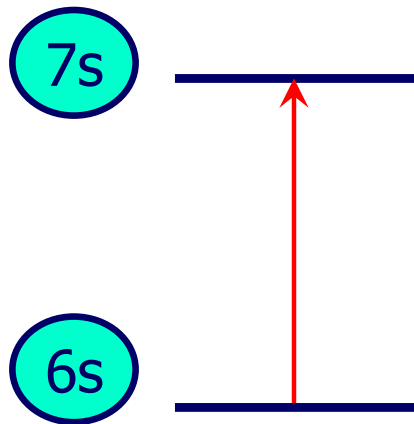


$$\frac{\text{Im}(E_{\text{PNC}})}{\beta} = \begin{cases} -1.6349(80) \text{ mV/cm} & \mathbf{1} \\ -1.5576(77) \text{ mV/cm} & \mathbf{2} \end{cases}$$

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

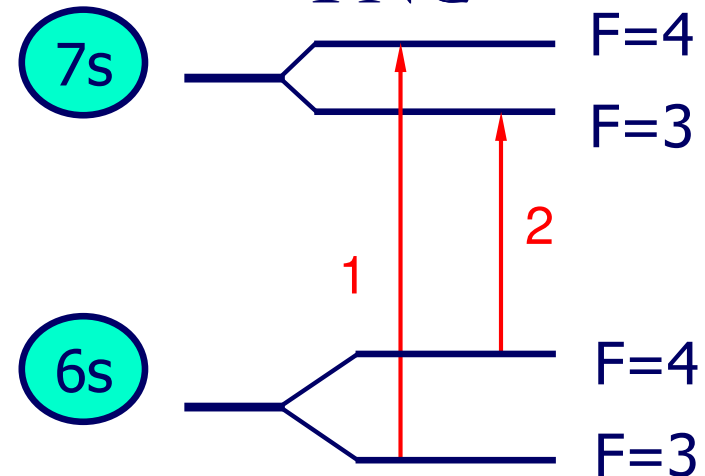


Average of 1 & 2

$$\frac{\text{Im}(E_{\text{PNC}}^{\text{si}})}{\beta} = -1.5935(56) \text{ mV/cm}$$

Weak Charge Q_W

NUCLEAR
SPIN-DEPENDENT
PNC



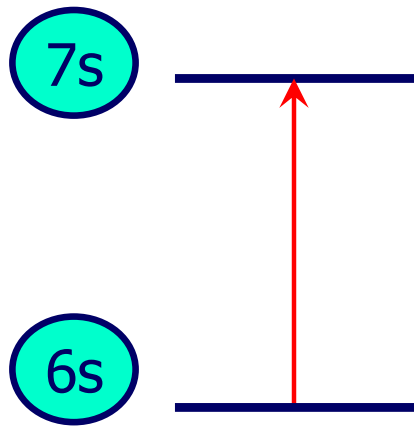
Difference of 1 & 2

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

Nuclear anapole moment

Analysis of Cs PNC experiment

NUCLEAR
SPIN-INDEPENDENT
PNC



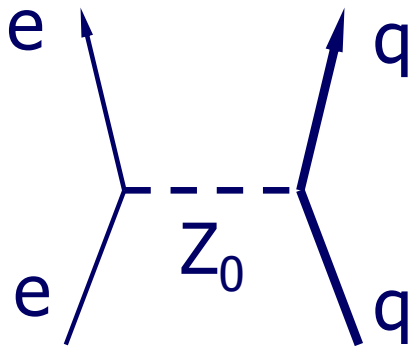
Average of 1 & 2

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

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)

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

Neutron density function

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

Extraction of weak the charge:

Theoretical calculation of
PNC amplitude

Measured value $\longrightarrow E_{PNC} = E_{PNC}^{theory} Q_w^{inferred}$

Calculation of PNC amplitude

1. Main part – Coulomb interactions

Electric-dipole matrix elements

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

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

REDUCING THEORY UNCERTAINTY: WHY IS IT SO DIFFICULT?

$$|\Psi_v\rangle = \Omega |\Psi_v^{(0)}\rangle$$

Exact wave function

Many-body operator,
describes excitations from lowest-order

Dirac-Hartree-Fock
wave function (lowest order)

Cs: 55 electrons \longrightarrow **55-fold excitations to get exact wave function**

Even for 100 function basis set $\longrightarrow 100^{55}$

Approximate methods: perturbation theory does not converge well,
Need to use all-order methods (coupled-cluster method and correlation potential method)

Coupled-cluster method (CCSD)

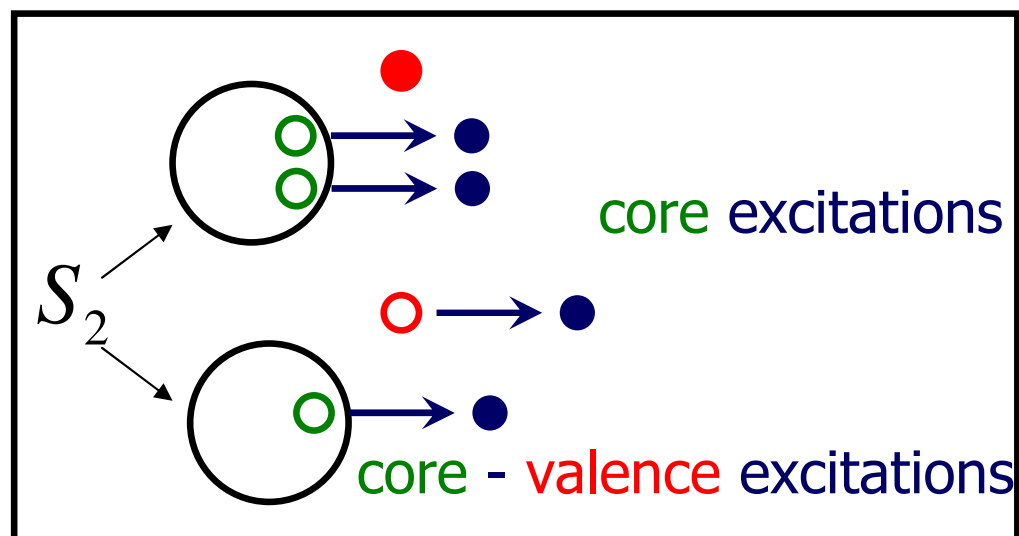
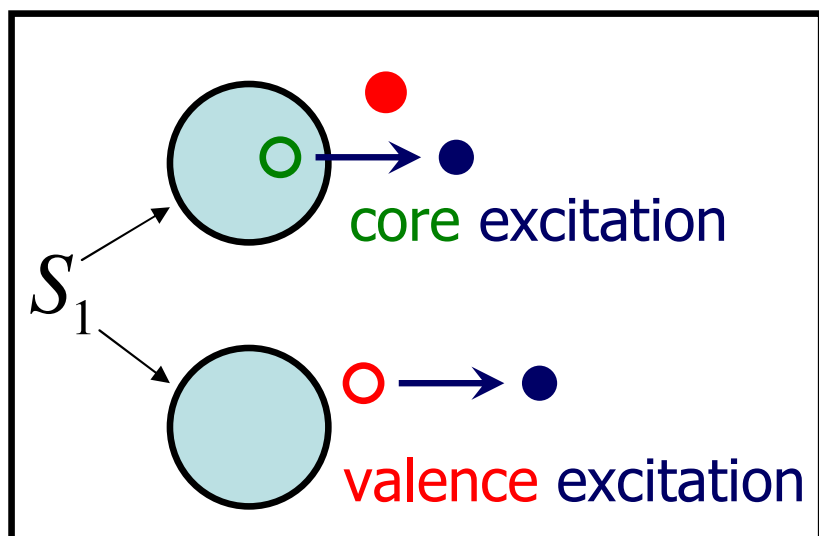
$$|\Psi_v\rangle = \Omega |\Psi_v^{(0)}\rangle = \exp(S) |\Psi_v^{(0)}\rangle \longrightarrow \text{DHF wave function}$$

$$\exp(S_1 + S_2)$$

**CCSD single-double
coupled-cluster**

$$S_1 + S_2$$

LCCSD coupled-cluster



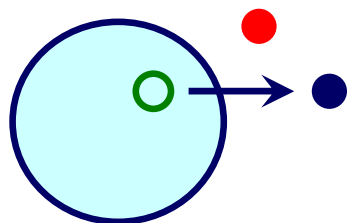
LCCSD ATOMIC WAVE FUNCTION

Lowest order

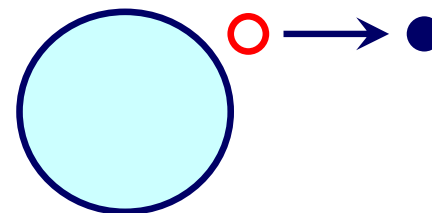


- core
- valence electron
- any excited orbital

Single-particle
excitations

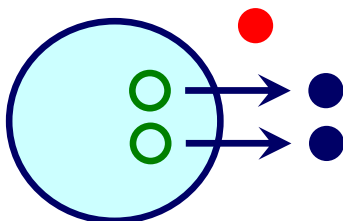


$$\sum_{ma} \rho_{ma} a_m^\dagger a_a |\Psi_v^{(0)}\rangle$$

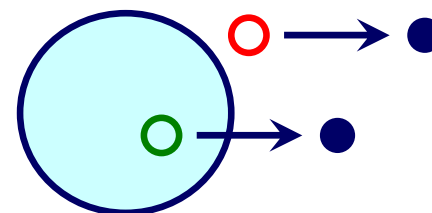


$$\sum_{m \neq v} \rho_{mv} a_m^\dagger a_v |\Psi_v^{(0)}\rangle$$

Double-particle
excitations



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



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

Actual implementation: problem 1

There are some many equations!

Need very accurate (large) basis sets for parity violation.

ρ_{mnab}

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

$m, n : \text{finite basis set} = (35 \times 13) \times (35 \times 13)$

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: problem 2

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: $n_{\max} = \mathbf{35}$, $l_{\max} = 6$

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

- Program has to be exceptionally efficient!

How to improve accuracy of CCSD?

1. Add more terms to the all order wave-function

Non-linear terms

Triple excitations

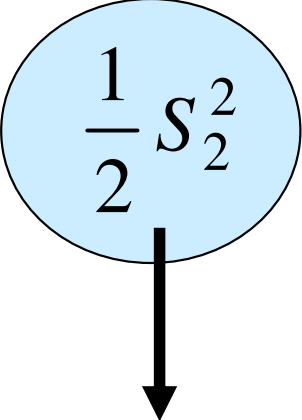
$$\frac{1}{2}(S_1^2 + 2S_1S_2 + S_2^2)$$

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

S_3

2. Restore complete 4th order for matrix elements

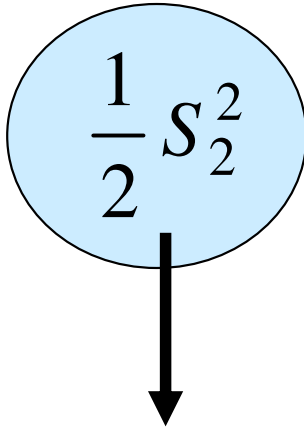
Non-linear terms





Contract operators by Wick's theorem

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

Non-linear terms

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


Contract operators by Wick's theorem

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



800 TERMS!



Codes that write formulas

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

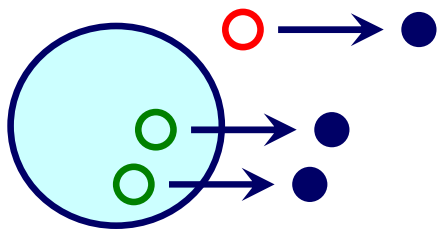
Solution: **develop analytical codes** that do all the work for you!

Input: ASCII input of terms of the type

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

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

Triple excitations



- core
- valence electron
- any excited orbital

$$\sum_{mnrab} \rho_{mnr\textcolor{red}{v}\textcolor{green}{ab}} a_m^\dagger a_n^\dagger a_r^\dagger \textcolor{green}{a}_a \textcolor{green}{a}_b \textcolor{red}{a}_v \left| \Psi_{\textcolor{red}{v}}^{(0)} \right\rangle$$

Problem 1: too many excitation coefficients $\rho_{mnr\textcolor{red}{v}\textcolor{green}{ab}}$

Problem 2: increased complexity of equations .

Triple excitations

Problem: too many excitation coefficients ρ_{mnrvab} .

Doubles:

ρ_{mnab}

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

$m, n : \text{finite basis set} = (35 \times 13) \times (35 \times 13)$

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 !

Codes that write formulas



Codes that write codes

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!

RESULTS FOR ALKALI-METAL ATOMS: E1 MATRIX ELEMENTS (A.U.)

	Na 3p _{1/2} -3s	K 4p _{1/2} -4s	Rb 5p _{1/2} -5s	Cs 6p _{1/2} -6s	Fr 7p _{1/2} -7s
All-order	3.531	4.098	4.221	4.478	4.256
Experiment	3.5246(23)	4.102(5)	4.231(3)	4.489(6)	4.277(8)
Difference	0.18%	0.1%	0.24%	0.24%	0.5%

Experiment **Na,K,Rb**: U. Volz and H. Schmoranzner, Phys. Scr. T65, 48 (1996),
Cs: R.J. Rafac et al., Phys. Rev. A 60, 3648 (1999),
Fr: J.E. Simsarian et al., Phys. Rev. A 57, 2448 (1998)

Theory M.S. Safronova, W.R. Johnson, and A. Derevianko,
 Phys. Rev. A 60, 4476 (1999)

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)
- 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

1989 – 2003: Summary of the PNC calculations

-0.902, -0.908 (-0.905 average) Blundell et al. (1992)
-0.908 Dzuba et al. (1989)

-0.909 Safronova & Johnson (1999)
-0.905 Kozlov et al. (2001)
-0.908 Dzuba et al. (2002) **0.5% uncertainty**

Units: $i|e|a_B(-Q_W / N) \times 10^{11}$

-0.6% Breit correction
-0.2(1)% neutron skin correction
+0.4% vacuum polarization
-0.8% radiative corrections

← (Several works for all corrections)

Determination of Q_W : 1997 - 2003

Wood et al. (1997) $\text{Im}(E_{\text{PNC}})/\beta$	-72.11(29) _{expt} (89) _{theor}	1 σ
Bennett & Wieman (1999) Measurement of β	-72.06(29) _{expt} (34) _{theor}	2.5 σ
Derevianko (2000,2002) Calculation of Breit correction	-72.61(29) _{expt} (34/73) _{theor}	1.3 σ /0.7 σ
Dzuba et al. (2000) Calculation of Breit correction	-72.42(29) _{expt} (74) _{theor}	1.5 σ /no dev.
Kozlov et al. (2001) Calculation of E_{PNC} , Breit correction	-72.5(7)	no deviation
Johnson et al. (2001) Calculation of vacuum pol. corr.	-72.12(29) _{expt} (34/74) _{theor}	2.2 σ /1.2 σ
Milstein & Sushkov (2002) Calculation of vacuum pol. corr.		2.2 σ
Vasilyev et al. (2002) Measurement of 6s-7p trans., β	-72.65(49)	1.1 σ
Dzuba et al. (2002) E_{PNC}	-72.16(29) _{expt} (36) _{th}	2 σ
Flambaum & Kuchiev (2002)	-72.71(29) _{expt} (36) _{th}	no deviation
Milstein et al. (2003) self-energy & vertex corr.	-72.81(29) _{expt} (36) _{th}	0.6 σ

Summary of the PNC amplitude calculations

Coulomb interaction		Porsev et al., PRL 102, 181601 (2009)
Main part, n = 6 - 9	0.8823(18)	
Tail	0.0175(18)	
Total	0.8998(25)	
Corrections		
Breit	-0.0054(5)	Derevianko, PRL 85, 1618 (2000)
QED	-0.0024(3)	Shabaev et al., PRL 94, 213002 (2005)
Neutron skin	-0.0017(5)	Derevianko, PRA 65, 012016 (2000)
e-e weak interactions	0.0003	Blundell et al., PRL 65, 1411 (1990)
Final	0.8906(26)	Porsev et al., PRL 102, 181601 (2009)

Units: $i|e|a_B(-Q_W / N) \times 10^{11}$

Cs PNC: Comparison with the standard model

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

Most current result for Cs PNC Expt/Theory:

Atomic physics [2] :

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

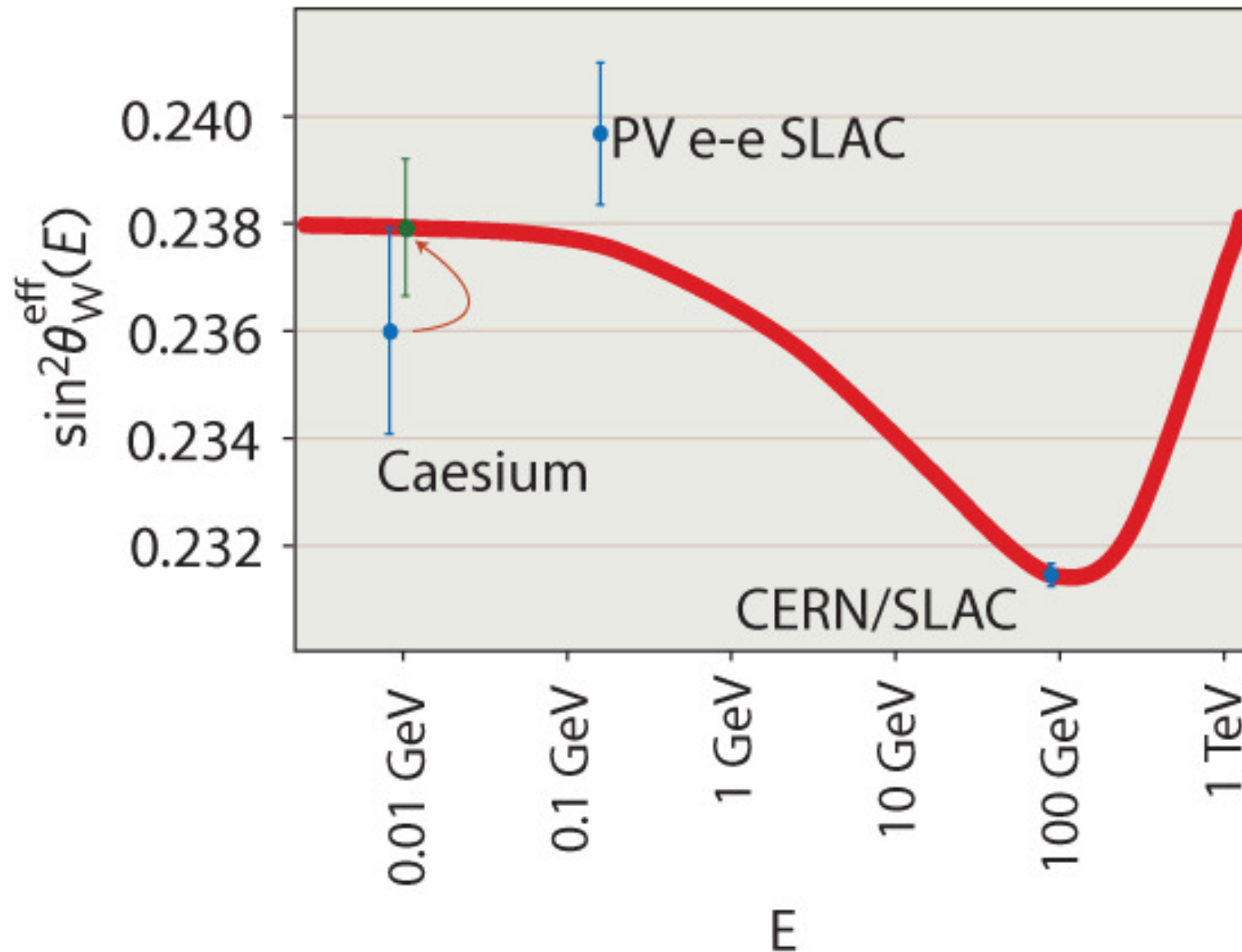
No deviation from the Standard Model

[1] C. Amsler et al. (Particle 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 \rightarrow 100 GeV



Adopted from Czarnecki & Marciano, Nature (2005)

Probing new physics

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

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

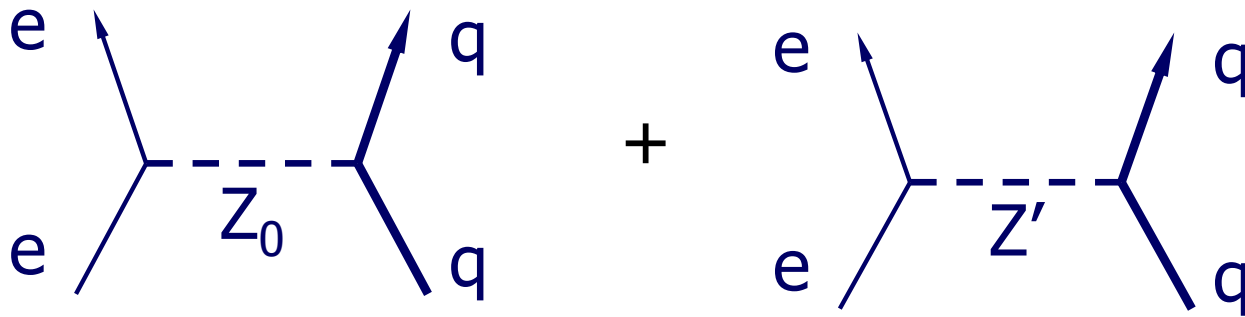
Present result [2]: $|S| < 0.45$

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'_x in SO(10) GUT, Marciano & Rosner

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

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]

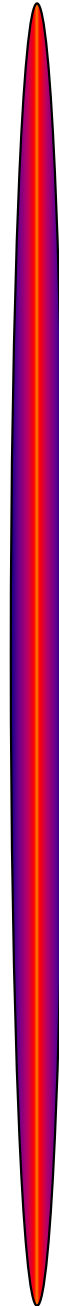
$$M_{Z'_x} > 0.82 \text{ TeV} / c^2$$

[1] S. G. Porsev, K. Beloy and A. Derevianko, PRL 102, 181601 (2009)

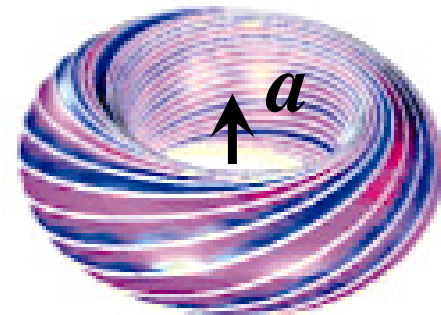
[2] T. Aaltonen et al., Phys. Rev. Lett. 99, 171802 (2007)

Parity violation in atoms

The other part
of the story

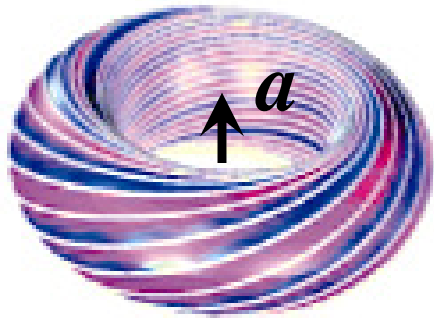


NUCLEAR
SPIN-DEPENDENT
PNC:
STUDY OF PNC
IN THE NUCLEUS



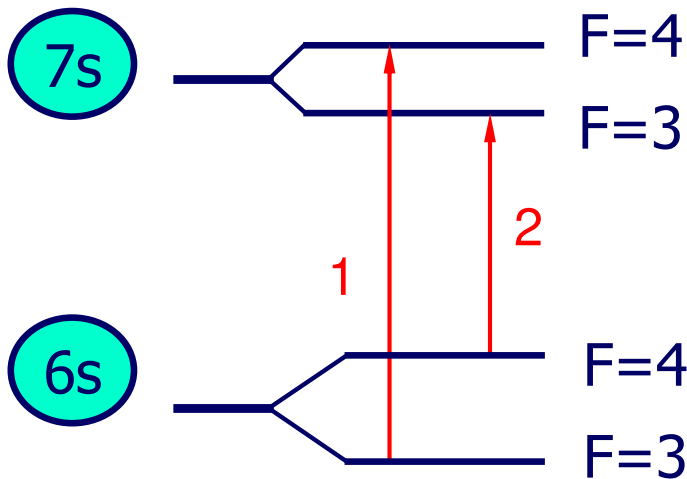
Nuclear anapole
moment

Spin-dependent parity violation: Nuclear anapole moment



Parity-violating nuclear moment

Valence nucleon density

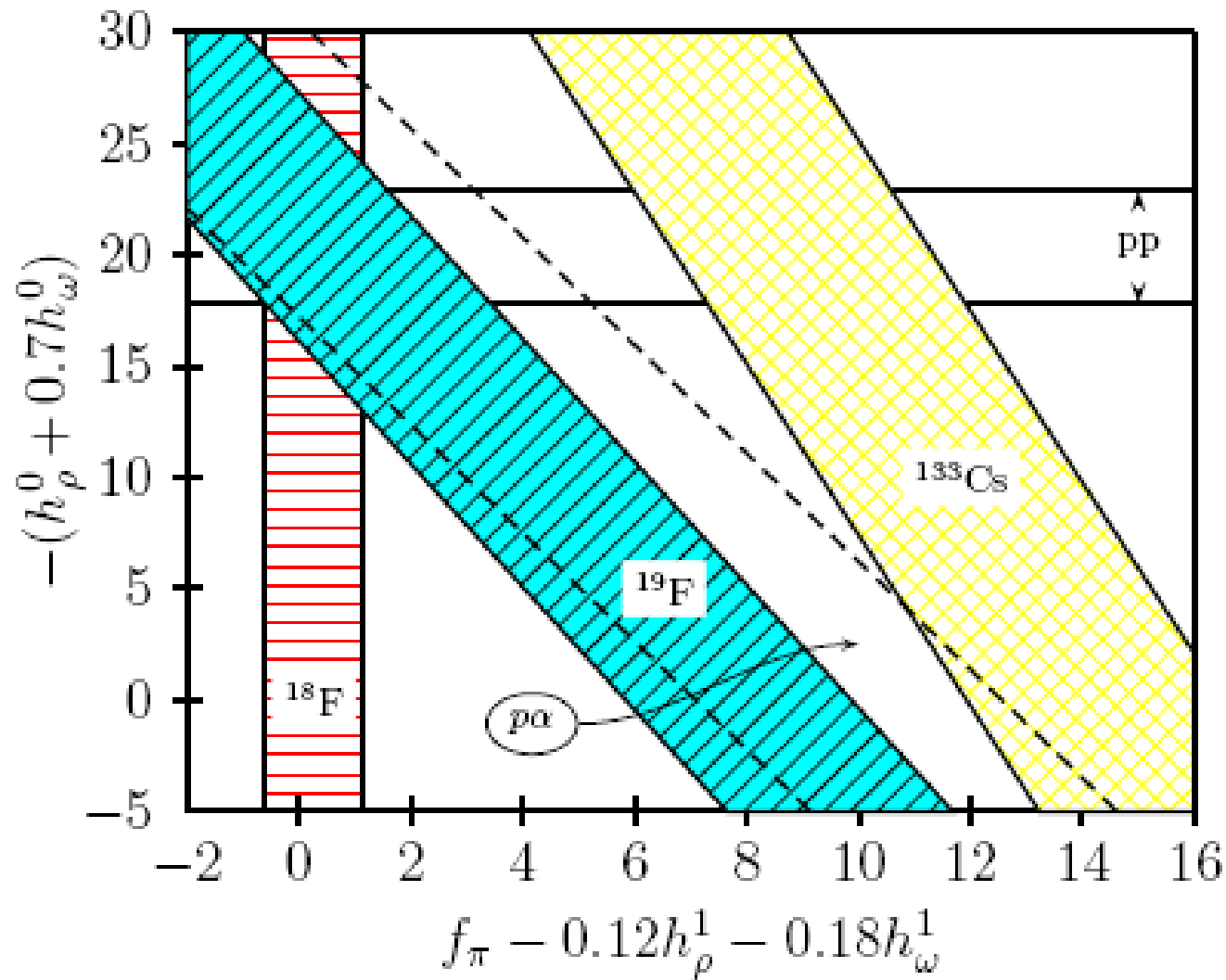


$$H_{\text{PNC}}^{(a)} = \frac{G_F}{\sqrt{2}} \kappa_a \mathbf{a} \cdot \mathbf{I} \rho_v(r)$$

Anapole moment

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

Constraints on nuclear weak coupling constants

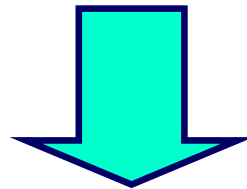


Nuclear anapole moment?

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?

$$K = 0.117(16)$$



Incomplete correlation calculation of spin-dependent PNC amplitude?

More spin-dependent PNC effects

$$K = K_a + K_2 + K_{\text{hf}}$$

(V_e, A_N)
interaction

Weak-hyperfine
interference term

Same Hamiltonian as
anapole moment term
with $K_a \Rightarrow K_2$

This term does not reduce to the
same interaction but “effective”
constant K_{hf} can be calculated.

New all-order (CCSD) calculation of spin-dependent PNC

Electric-dipole matrix elements

$$E_{\text{PNC}}^{(2,a)} = \mathcal{A}_1 \sum_{j \neq v} \frac{\langle 7s || d || j \rangle \langle j || H_{\text{PNC}}^{(2,a)} || 6s \rangle}{E_{6s} - E_j} + \mathcal{A}_2 \sum_{j \neq w} \frac{\langle 7s || H_{\text{PNC}}^{(2,a)} || j \rangle \langle j || D || 6s \rangle}{E_{7s} - E_j}$$

PNC matrix elements

First four terms in the sums are replaced by
all-order matrix elements
1% accuracy is expected

Nuclear anapole moment: Test of hadronic weak interactions

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:

$$k = 0.107(16)^* \text{ [1\% theory accuracy]}$$

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

NEED NEW
EXPERIMENTAL
PNC
STUDIES

WANTED!

PERIODIC TABLE

Atomic Properties of the Elements

NIST

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

Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
	IA	IIA	IIIB	IVB	VB	VIB	VII	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	IIIA
Period	1 H Hydrogen 1.00794 $1s^1$	2 He Helium 4.002602 $1s^2$	3 Li Lithium 6.941 $1s^2 2s^1$	4 Be Beryllium 9.012182 $1s^2 2s^2$	5 B Boron 10.811 $1s^2 2s^2 2p^1$	6 C Carbon 12.0107 $1s^2 2s^2 2p^2$	7 N Nitrogen 14.0067 $1s^2 2s^2 2p^3$	8 O Oxygen 15.9994 $1s^2 2s^2 2p^4$	9 F Fluorine 18.9984032 $1s^2 2s^2 2p^5$	10 Ne Neon 20.1797 $1s^2 2s^2 2p^6$	11 Na Sodium 22.989770 $[Ne]3s^1$	12 Mg Magnesium 24.3050 $[Ne]3s^2$	13 Al Aluminum 26.981538 $[Ne]3s^2 3p^1$	14 Si Silicon 28.0855 $[Ne]3s^2 3p^2$	15 P Phosphorus 30.973761 $[Ne]3s^2 3p^3$	16 S Sulfur 32.065 $[Ne]3s^2 3p^4$	17 Cl Chlorine 35.453 $[Ne]3s^2 3p^5$	18 Ar Argon 39.948 $[Ne]3s^2 3p^6$
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All-order
Correlation potential

CI+MBPT

■ Solids
■ Liquids
■ Gases
■ Artificially Prepared

Atomic Number	Ground-State
58	$1G_4$
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)

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 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

Conclusion

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.



GRADUATE STUDENTS:

Rupsi Pal*

Dansha Jiang*

Bindiya Arora*

Jenny Tchoukova*

Zhuriadna

Matt Simmons

*Graduated with a Ph.D.

COLLABORATORS

Michael Kozlov, PNPI, Russia

Sergei Porsev, PNPI, Russia

(presently research scholar at the University of Delaware)

Charles Clark, NIST

Ulyana Safronova, University of Nevada-Reno

Andrei Derevianko, University of Nevada-Reno

Ephraim Eliav, Tel Aviv University, Israel

Walter Johnson, University of Notre Dame