PRECISION TESTS WITH NEUTRAL-CURRENT COHERENT INTERACTIONS WITH NUCLEI

PARITY VIOLATION IN ATOMS

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An NSF Quantum Leap Challenge Institute

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https://thoriumclock.eu/

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REVIEWS OF MODERN PHYSICS, VOLUME 90, APRIL–JUNE 2018

Search for New Physics with Atoms and Molecules

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[2]Joint Quantum Institute, National Institute of Standards and Technology and the University of Maryland, College Park, Maryland, USA,
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This article reviews recent developments in tests of fundamental physics using atoms and molecules, including the subjects of parity violation, searches for permanent electric dipole moments, tests of the CPT theorem and Lorentz symmetry, searches for spatiotemporal variation of fundamental constants, tests of quantum electrodynamics, tests of general relativity and the equivalence principle, searches for dark matter, dark energy and extra forces, and tests of the spin-statistics theorem. Key results are presented in the context of potential new physics and in the broader context of similar investigations in other fields. Ongoing and future experiments of the next decade are discussed.

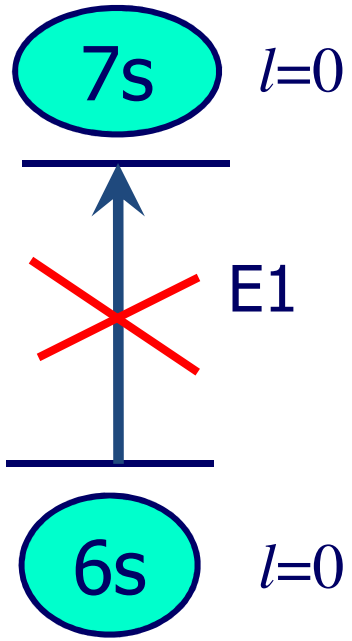
RMP 90, 025008 (2018)

Very wide scope of AMO new physics searches

- Precision tests of Quantum Electrodynamics
- Atomic parity violation
- Time-reversal violation: electric dipole moments and related phenomena
- Tests of the CPT theorem: matter-antimatter comparisons
- Lorentz symmetry tests
- Searches for light dark matter
- Search for variation of fundamental constants
- Searches for exotic forces
- General relativity and gravitation
- Search for violations of quantum statistics

Atomic Parity Violation

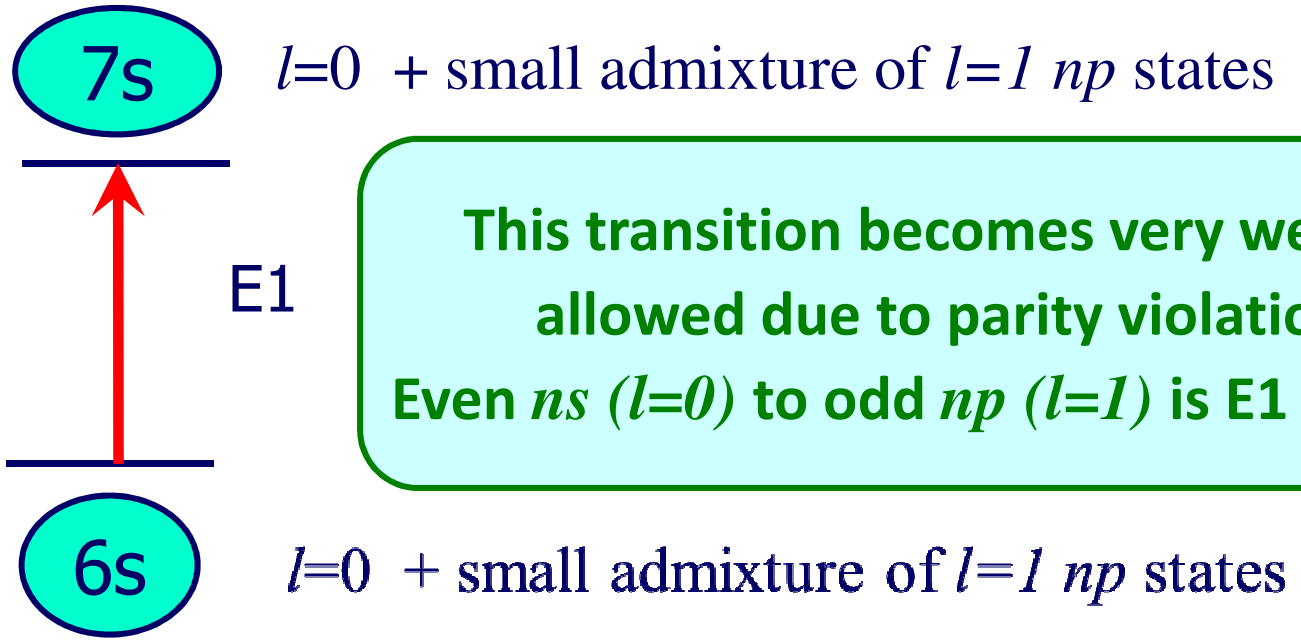
Cs atom



This electric dipole transition is forbidden
Even (l=0) to even (l=0) transition not allowed

Atomic Parity Violation

Cs atom + Parity Violation



To study parity violation in atoms: measure this transition amplitude.

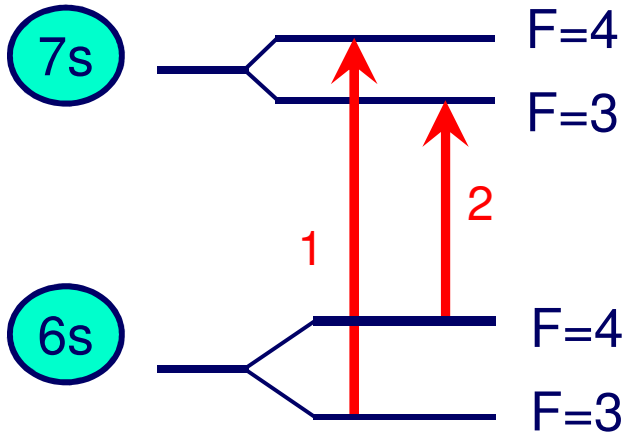
Atomic Parity Violation (APV)

Cs atom + Hyperfine Interactions

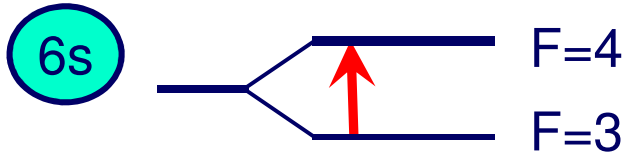
Cs nucleus: spin I=7/2

Both 6s and 7s states are split to two with total angular momenta F=3 and 4

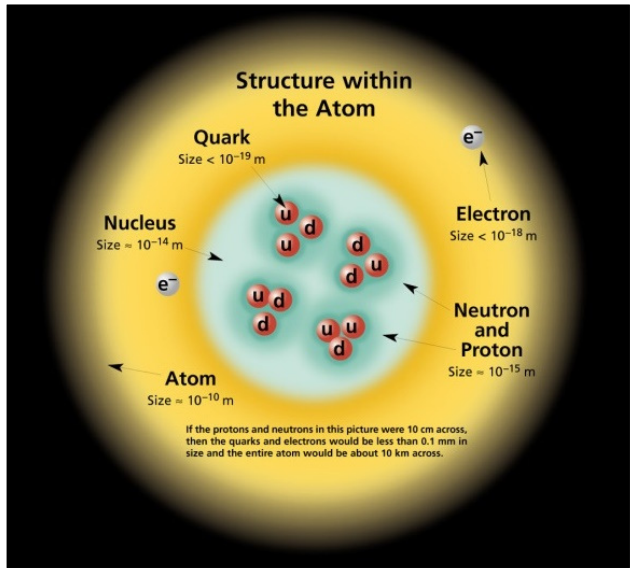
Optical transition scheme



Microwave transition scheme



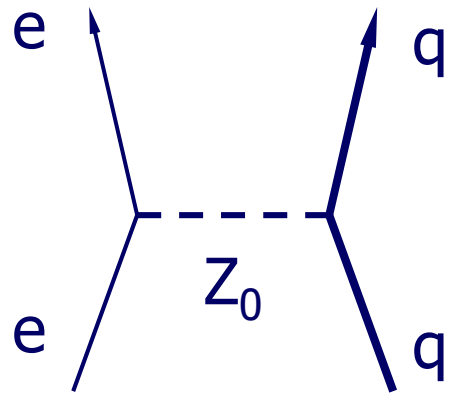
#1: Main Sources of Atomic Parity Violation: Z_0 exchange



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

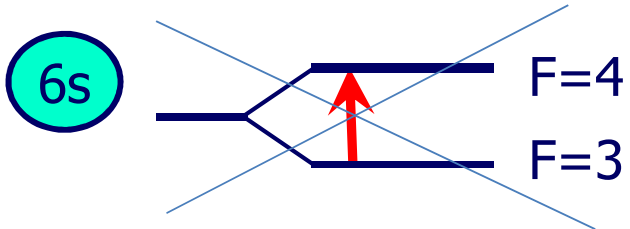
$$H_W = \frac{G_F}{\sqrt{2}}\left(\bar{e}\gamma_\mu\gamma_5 e\right)\left\{C_{1u}\,\bar{u}\gamma^\mu u + C_{1d}\,\bar{d}\gamma^\mu d\right\} + \ldots$$

Nuclear spin-independent interaction

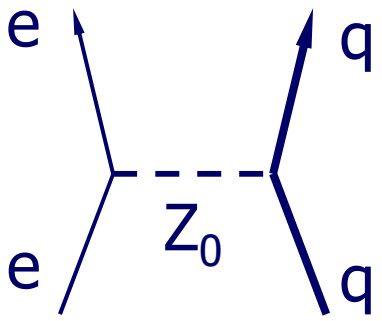


Optical transition scheme only!

No effect of the Z_0 exchange on the microwave transition scheme



What do we want extract from PNC amplitude?



Weak Charge Q_W

$$Q_W = -N + Z(1 - 4\sin^2\theta_W)$$

Neutron density function

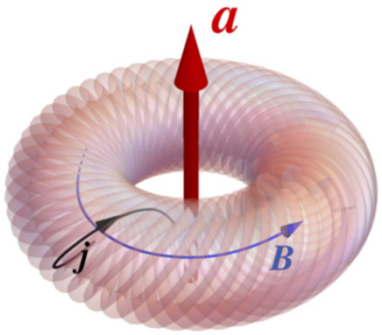
Electronic sector: $H^{(1)}_{PNC} = \frac{G_F}{2\sqrt{2}} Q_W \gamma_5 \rho(r)$

Extraction of weak the charge:

Theoretical calculation of PNC amplitude

Measured value → $E_{PNC} = E^{theory}_{PNC} Q^{inferred}_W$

#2: Main Sources of Atomic Parity Violation: Weak interactions inside the nuclei

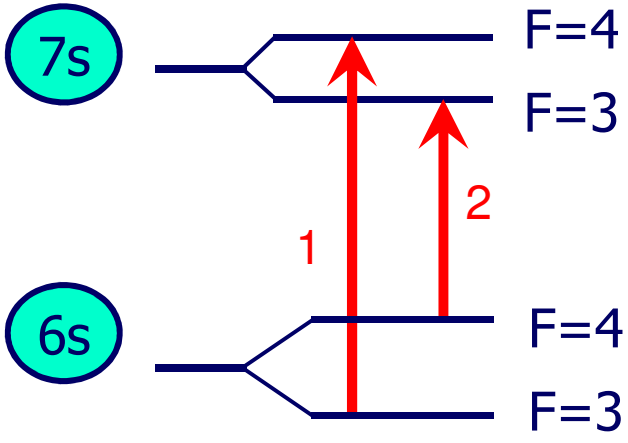


Parity-violating nuclear moment

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

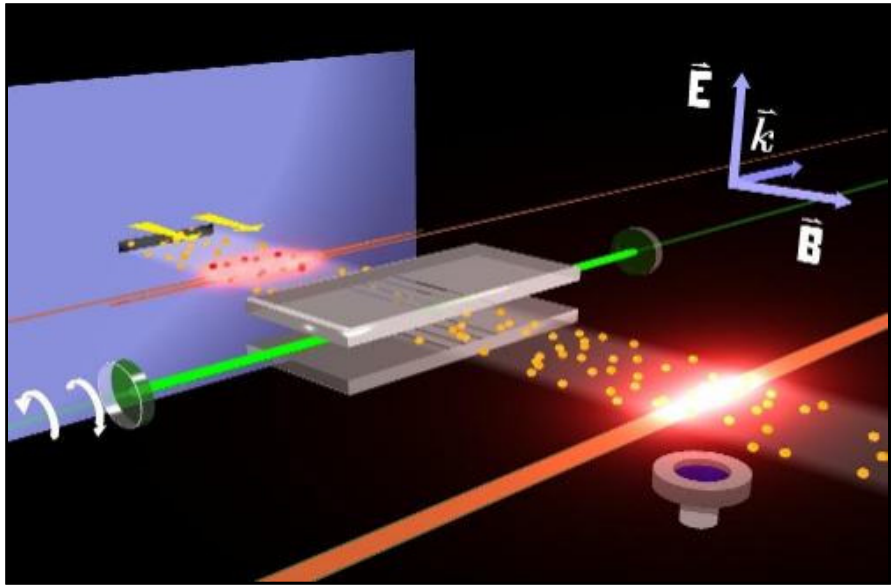


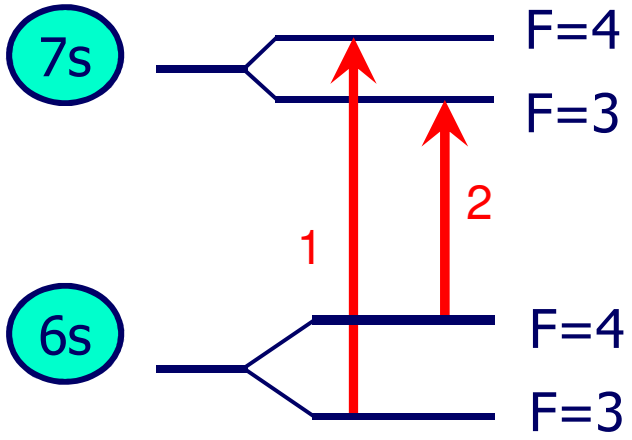
Need theory to extract anapole moment from experiment

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

Measurement of APV amplitude in cesium

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





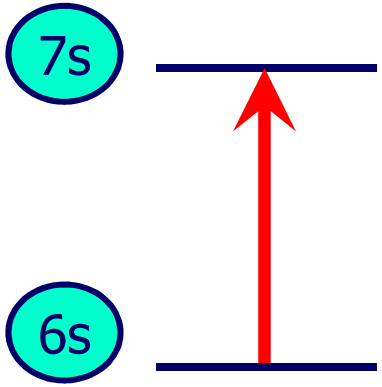
0.3% accuracy

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

NEED ATOMIC THEORY TO GET Q_W and ANAPOLE MOMENT FROM THIS EXPERIMENT

Analysis of Cs APV experiment

Nuclear
Spin - independent APV

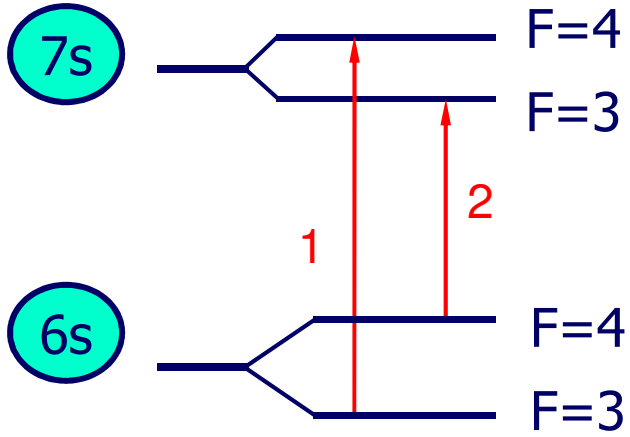


Average of 1 & 2

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

Weak Charge Q_W

Nuclear
spin-dependent APV



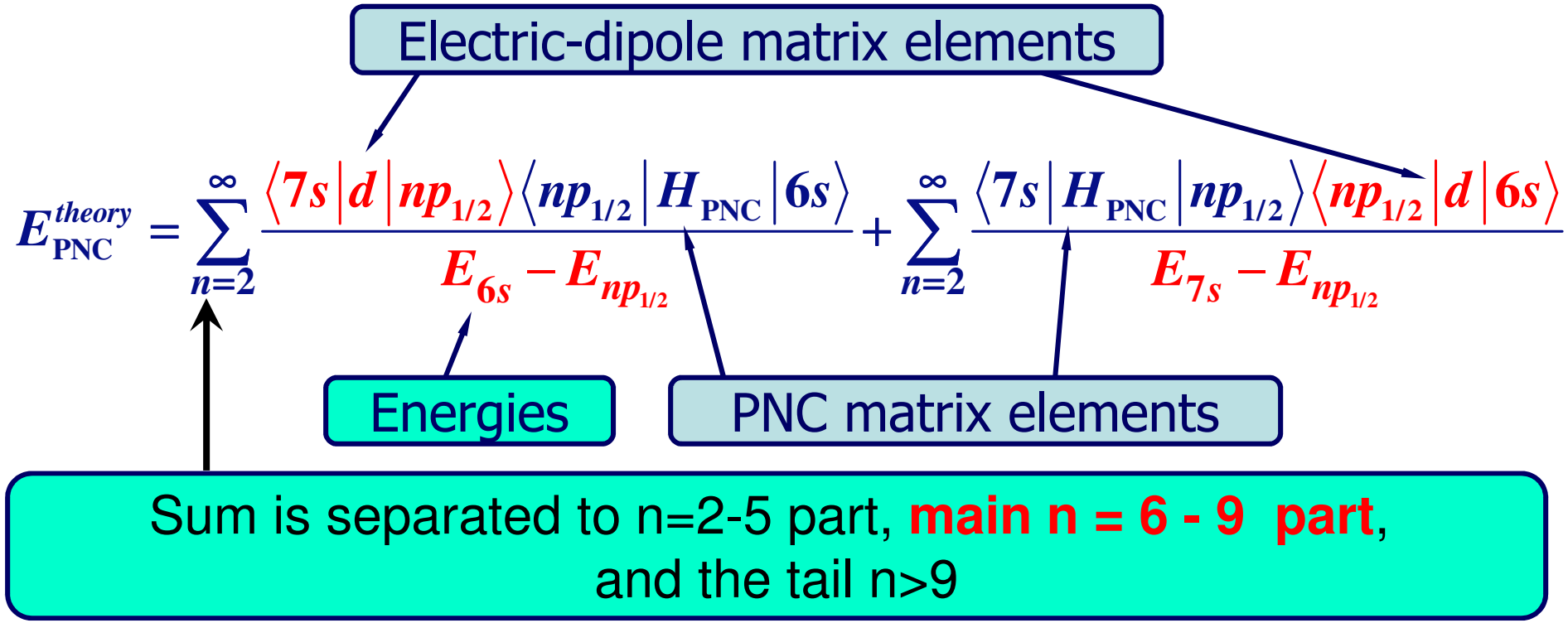
Difference of 1 & 2

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

Nuclear anapole moment

Calculation of PNC amplitude

1. Main part – Coulomb interactions



2. Other small corrections:

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

2009 Cs APV: Comparison with the Standard Model

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

2009 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)

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

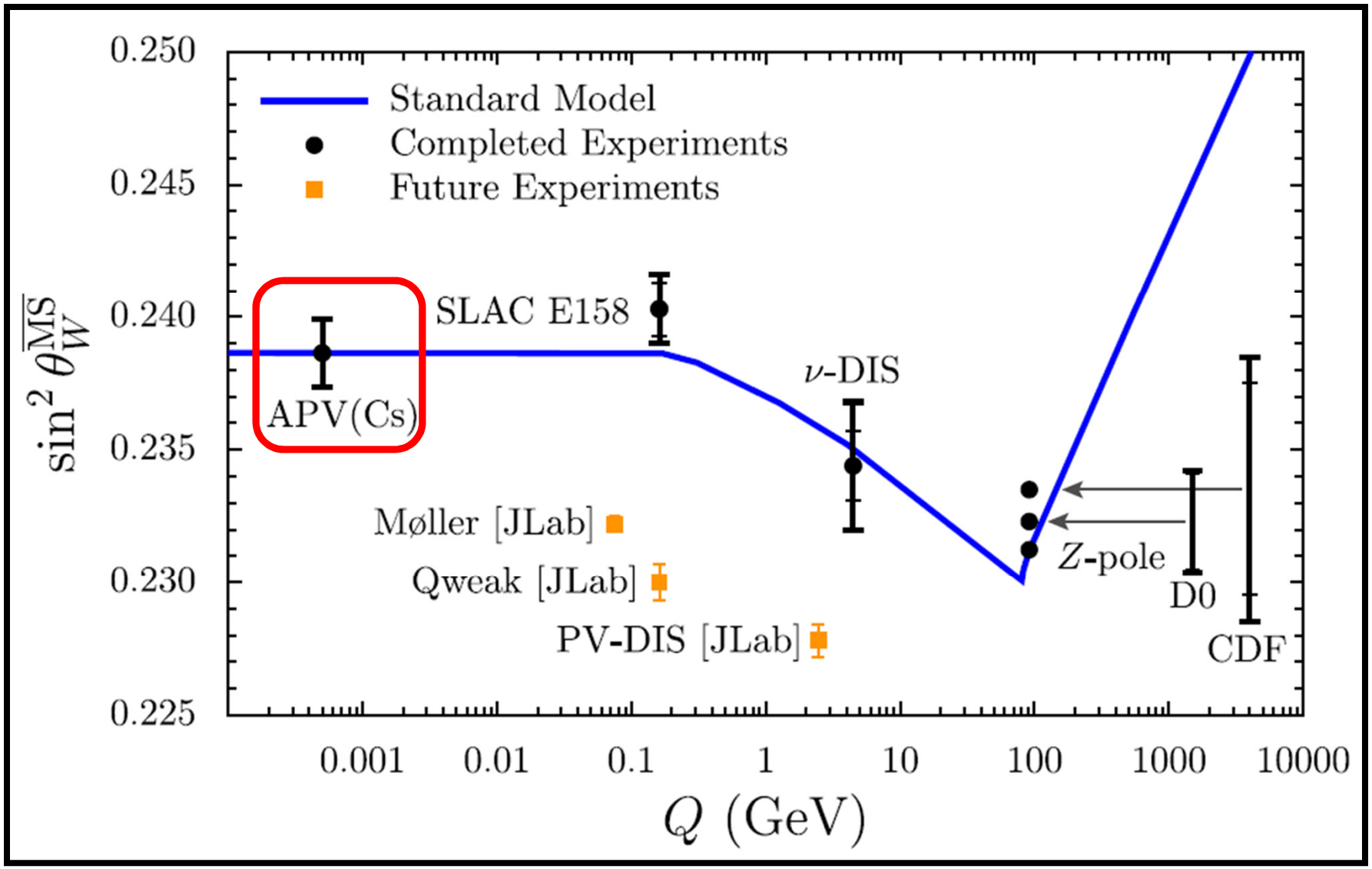


Figure is from Bentz *et al. Phys. Lett.* ***B693***, 462 (2010).

Cs APV : 2009 status

Contributions to PNC amplitude

Coulomb interaction		
Core, n = 2 - 5	-0.0020	
Main part, n = 6 - 9	0.8823(18)	
Tail	0.0195(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: $i|e|a_B(-Q_W/N)\times 10^{11}$

No deviation

Cs APV: 2012 corrections

V. A. Dzuba, J. C. Berengut, V.V. Flambaum, and B. Robets, *PRL* 109, 203003 (2012)

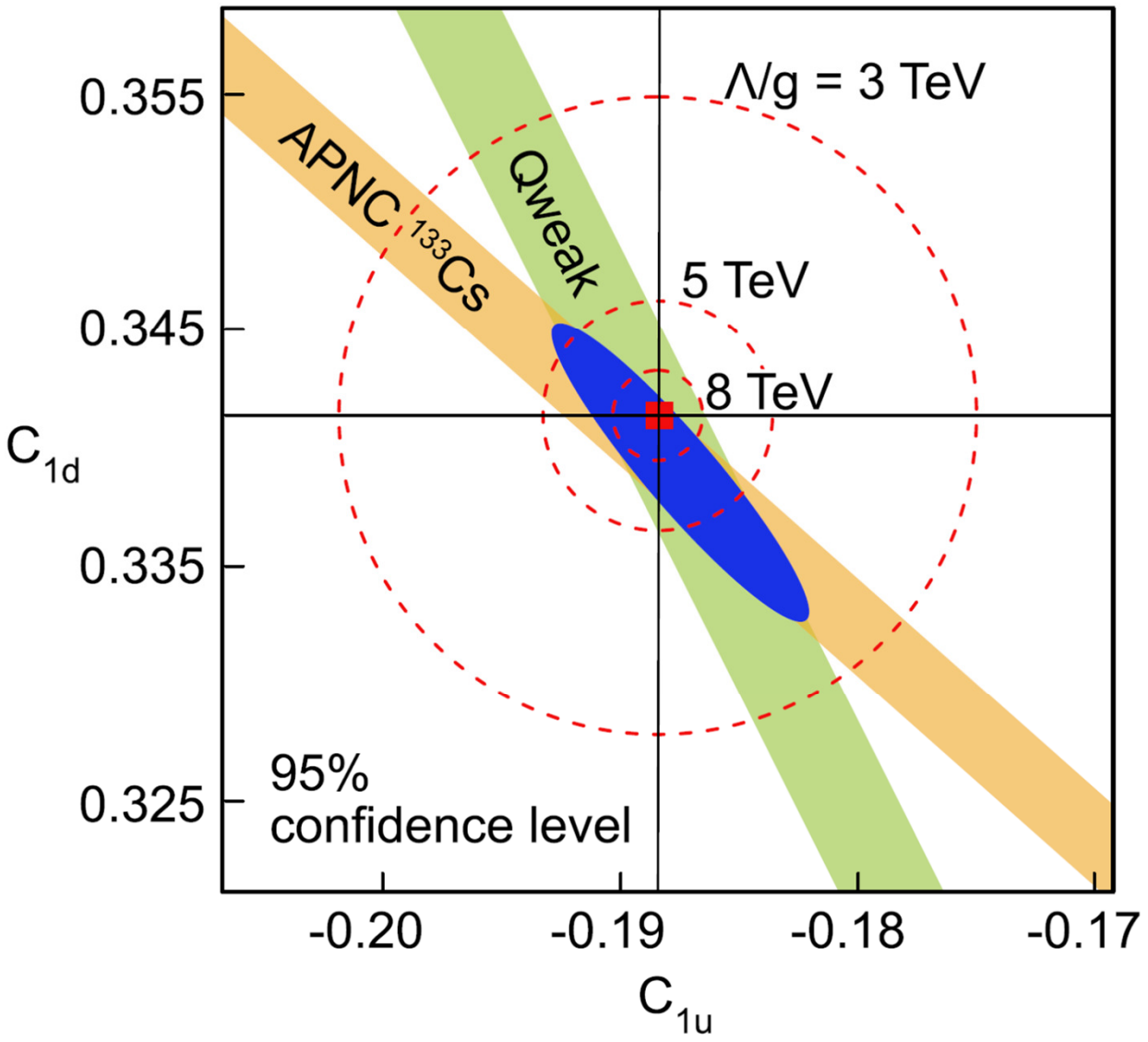
Coulomb interaction		
Core, n = 2 - 5	~~-0.0020~~	0.0018 0.44%change
Main part, n = 6 - 9	0.8823(18)	
Tail	~~0.0195(18)~~	0.0242(30) 0.58% change
Total	0.8998(25)	
Corrections		
Breit	-0.0054(5)	Derevianko, PRL 85, 1618 (2000)
QED	-0.0024(3)	Shabaev et al., PRL 94, 213002 (2005)
Neutron skin	-0.0017(5)	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)
Final	**0.8980(45)**	**Dzuba et al, PRL 109, 203003 (2012)**

Confirmed

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

1.5σ deviation

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

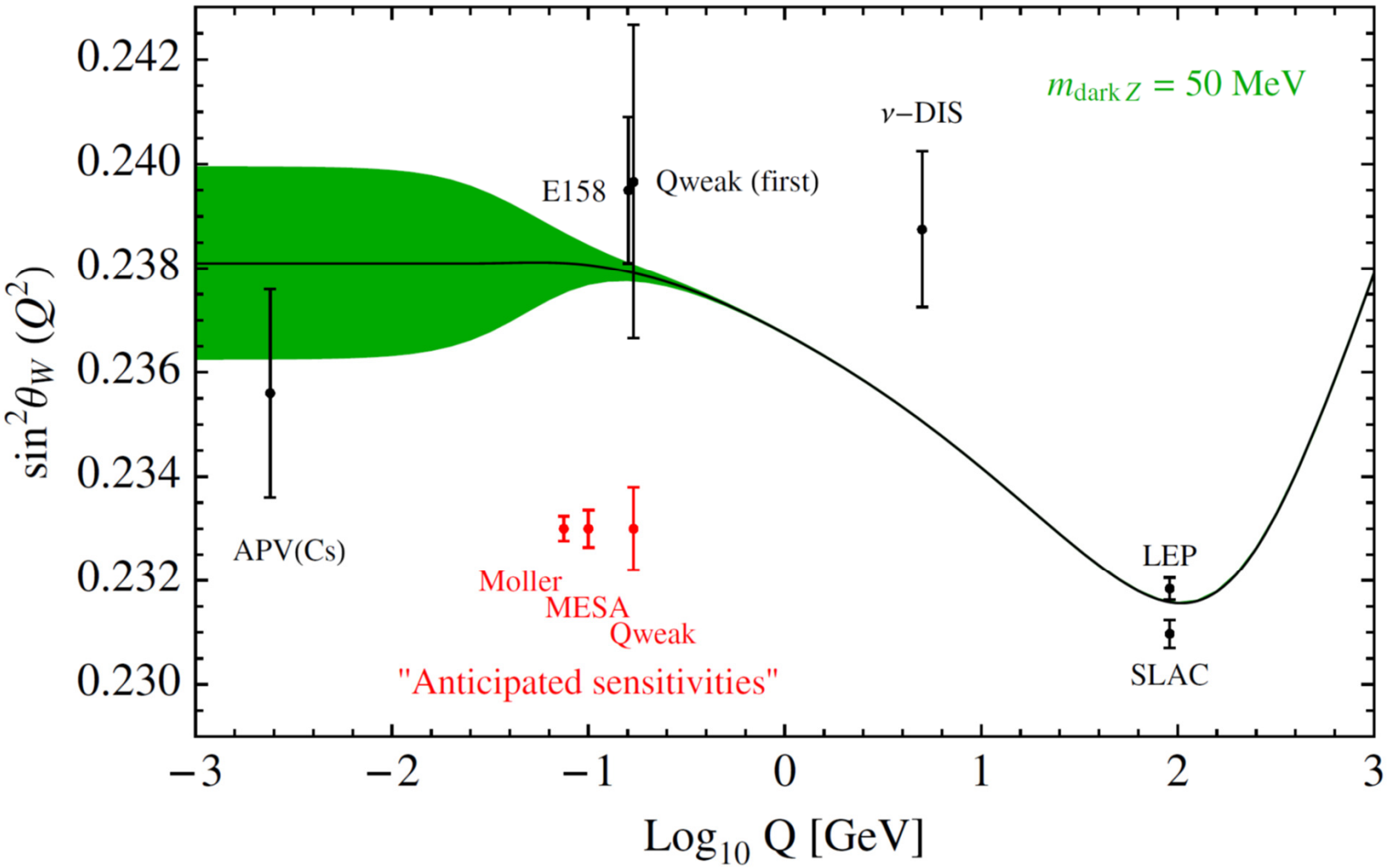


G. Gwinner and L. A. Orozco *Quantum Sci. Technol.* **7** 024001 (2022)

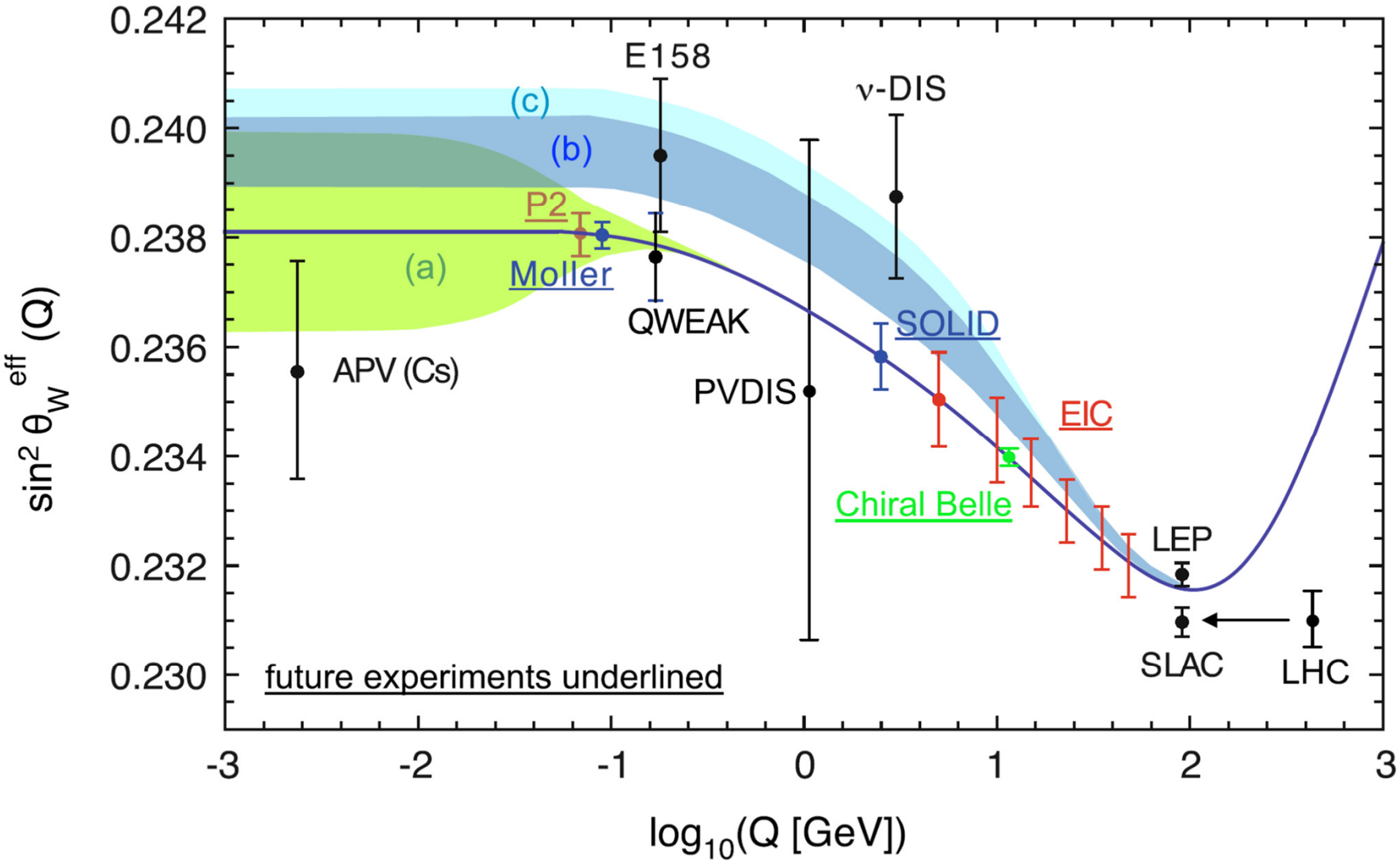
PHYSICAL REVIEW D **89,** 095006 (2014)

Muon $g-2$, rare kaon decays, and parity violation from dark bosons

Hooman Davoudiasl,[1] Hye-Sung Lee,[2,3] and William J. Marciano[1]



Past and future measurements of the Weinberg angle



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Neutron skin and Atomic parity violation

Atomic parity violation experiments with **chains** of isotopes

Neutron skin correction to APV amplitude

The relative neutron skin correction to the APV amplitude is independent from electronic structure and is given by:

$$\frac{\Delta E^{ns}_{\mathrm{PNC}}}{E_{\mathrm{PNC}}} = -\frac{3}{7}(\alpha Z)^2 \frac{\Delta R_{np}}{R_p}$$

Difference between rms radii of neutron and proton distributions

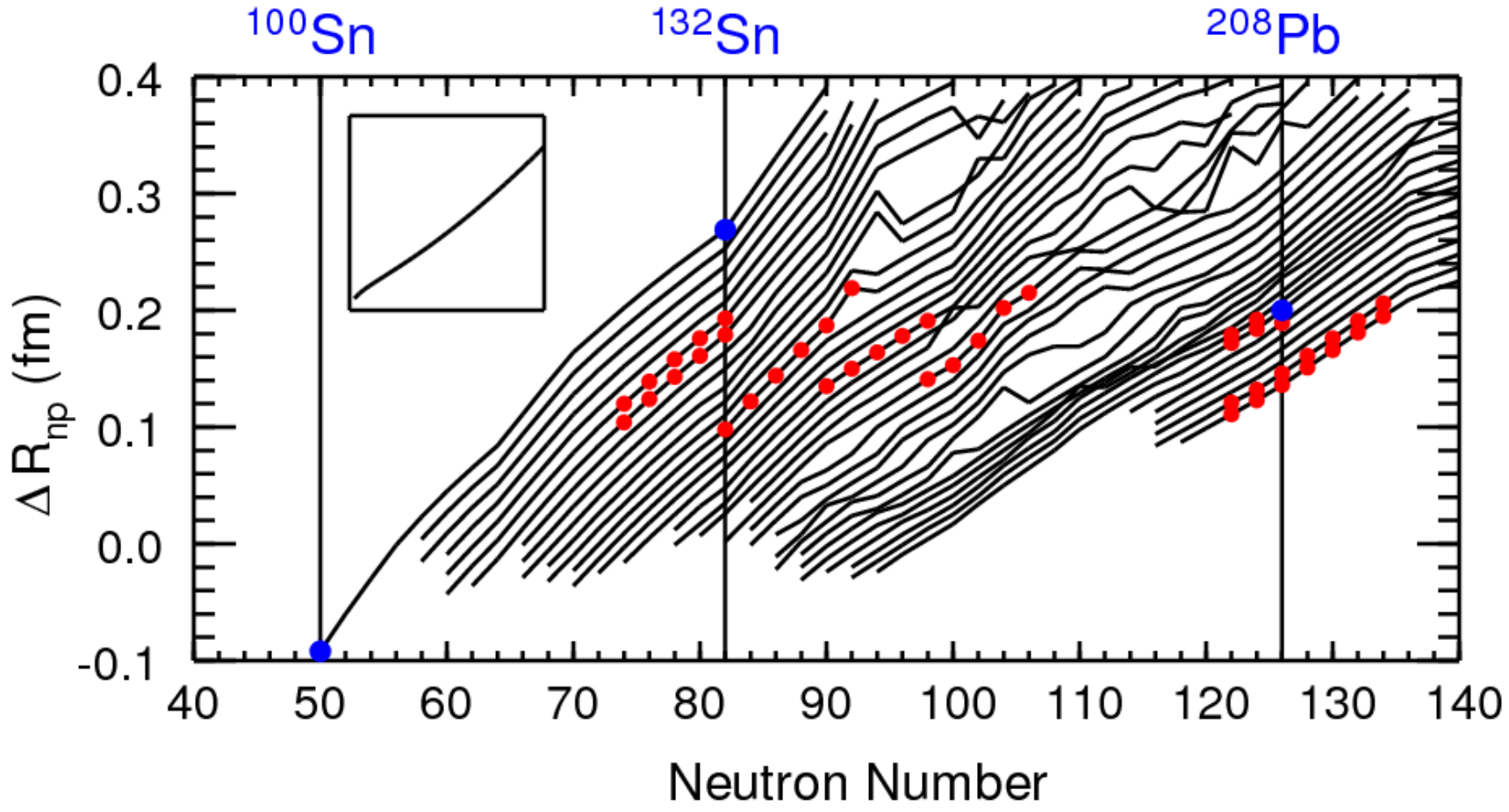
rms radius of proton distribution

Neutron skin correction is 0.2% for Cs, but **0.6% for Fr and Ra^+**

Therefore, neutron skin can be extracted from APV studies if their uncertainties are smaller than these values.

Pollock et al., PRC 46, 2587 (1992), Brown et al., PRC 79, 035501 (2009)

The neutron skin calculations, SkXs20



Different isotopes for a given element are connected by lines. The filled circles show nuclei of interest for atomic PV.

Alex Brown, 2008 PREX workshop, Brown et al., PRC 79, 035501 (2009)

Isotopic chain APV experiments

(1) APV isotopic chain experiments should allow to largely cancel dependence on atomic theory.

(2) Errors due to neutron skin in two isotopes are correlated. This should allows to **extract new physics** from such experiments

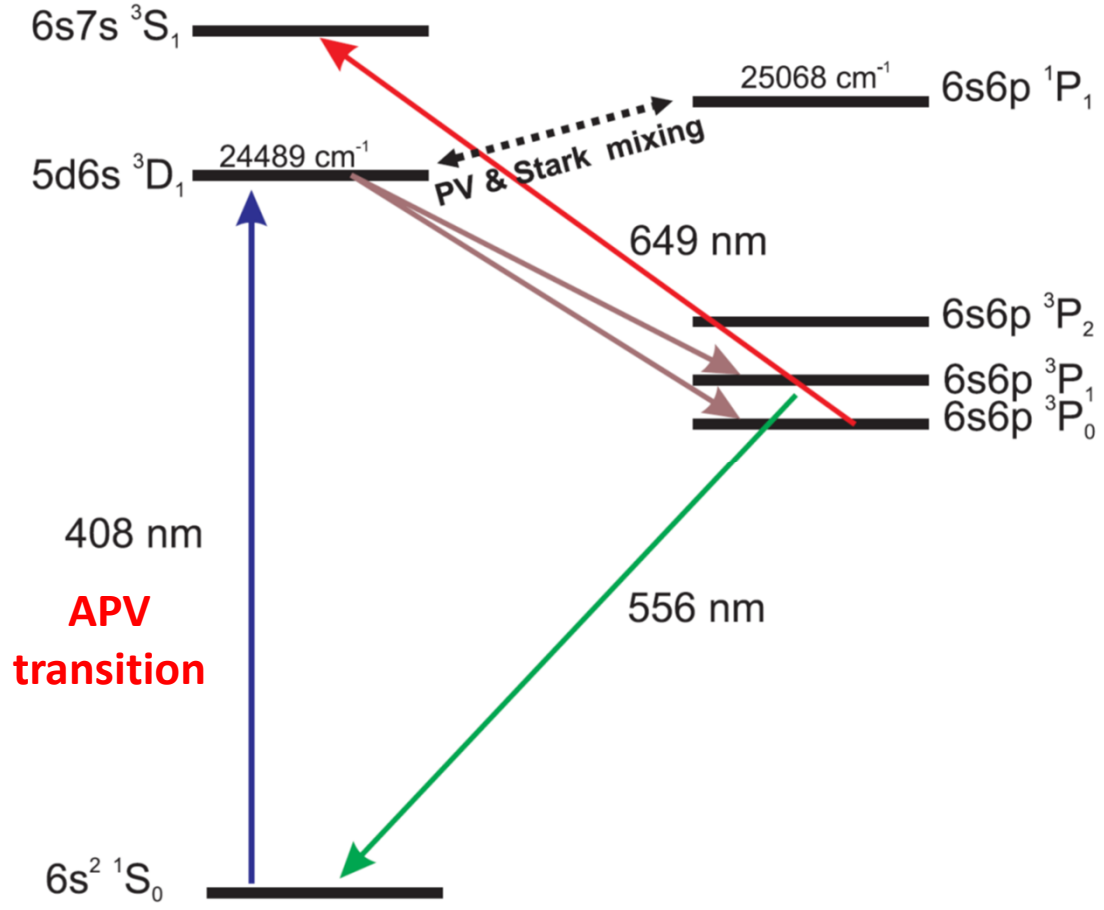
(3) The sensitivity to neutron skin effect is the largest for the lightest and heaviest pair of isotopes in the chain. It may be possible to **extract neutron skin** from such experiments.

ΔR_{np}

Atom	A	ΔR_{np}	$\Delta E^{ns}_{\mathrm{PNC}} / E_{\mathrm{PNC}}$
Yb (Z=70)	168	0.141(35)	-0.0031(8)
	176	0.215(67)	-0.0046(14)
Fr (Z=87)	209	0.121(36)	-0.0038(11)
	221	0.206(53)	-0.0064(16)

Brown et al., PRC 79, 035501 (2009)

Observation of a Large Atomic Parity Violation Effect in Ytterbium



K. Tsigutkin, D. Dounas-Frazer, A. Family, J. E. Stalnaker, V. V. Yashchuk, and D. Budker, Phys. Rev. Lett. **103**, 071601 (2009)

The parity-violating amplitude is found to be 2 orders of magnitude larger than in cesium.

$$A^{\mathrm{PV}}_{FMF'M'} = i\zeta_{FF'}(-1)^q \mathcal{E}_q \langle F, M, 1, -q | F', M' \rangle$$

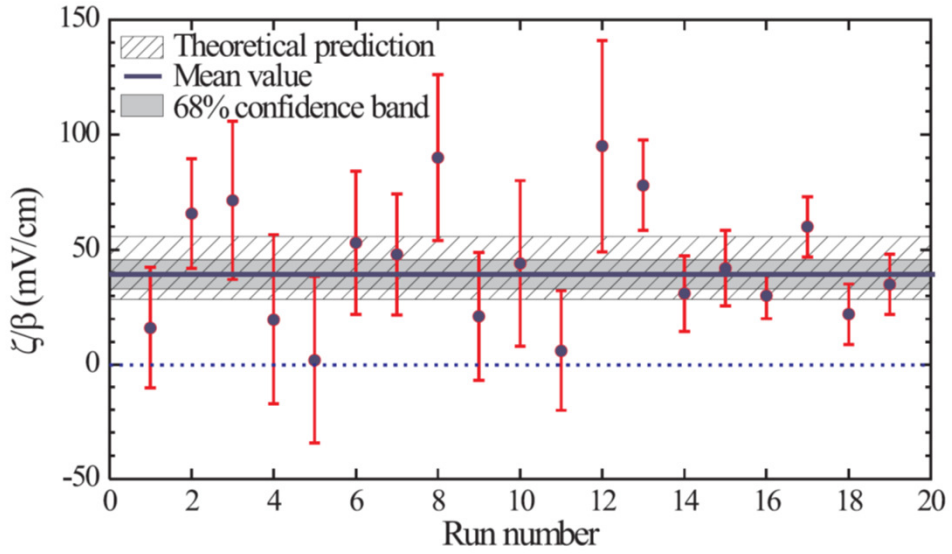
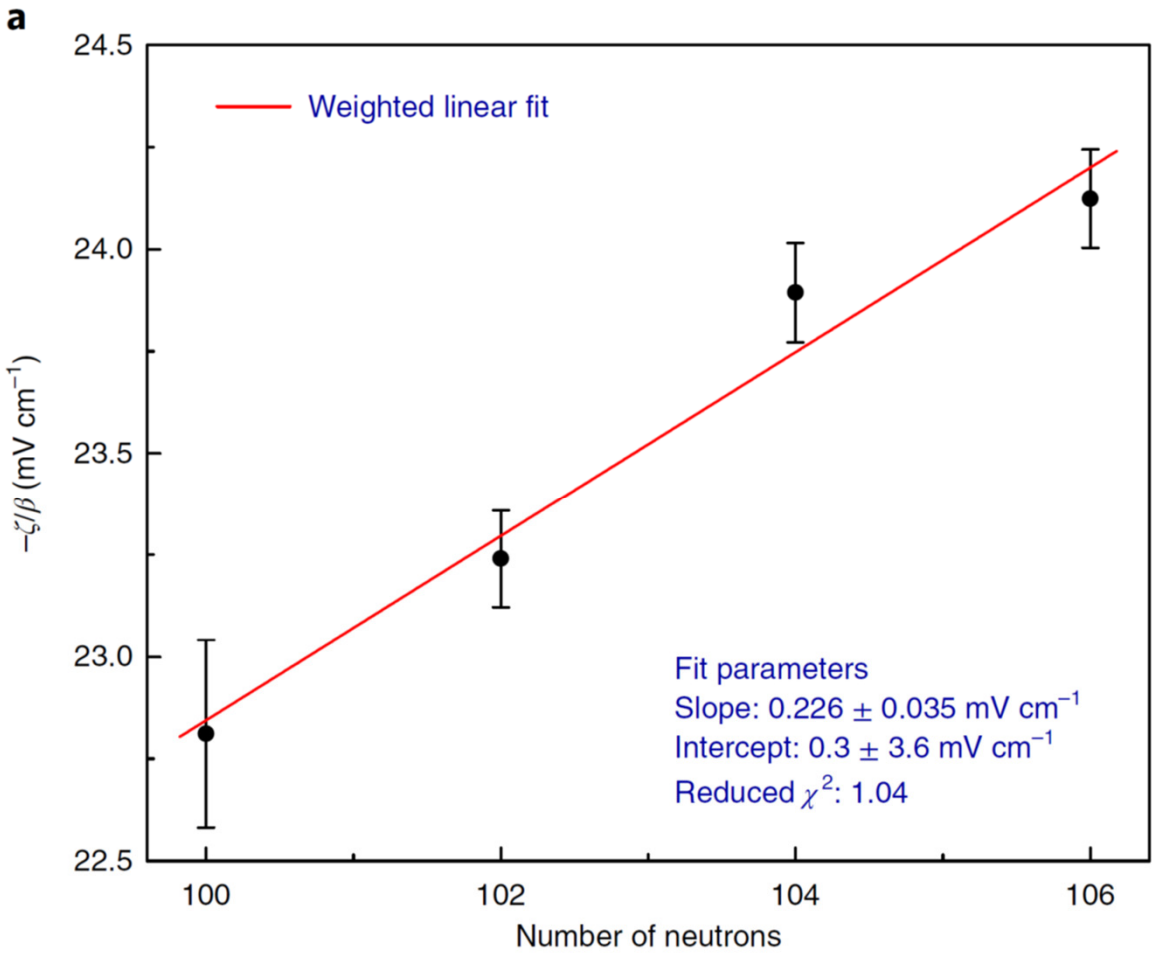


FIG. 5 (color online). The PV-interference parameter ζ/β. Mean value: $39(4)_{\mathrm{stat}}(5)_{\mathrm{syst}}$ mV/cm, $|\zeta| = 8.7 \pm 1.4 \times 10^{-10} ea_0$. The 68% confidence band includes both the statistical and the systematic uncertainties.

Isotopic variation of parity violation in atomic ytterbium



APV effect was measured in four nuclear-spin-zero isotopes (^{170}Yb, ^{172}Yb, ^{174}Yb and ^{176}Yb, with abundances of 3.1, 21.9, 31.8 and 12.7%, respectively).

The single-isotope accuracy in this experiment is approximately 0.5% for three of the Yb isotopes measured.

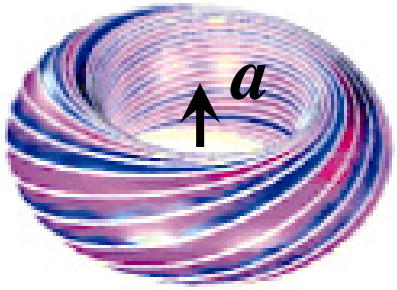
Further upgrades will enhance the measurement sensitivity to a level that allows high-precision isotopic comparison to probe the neutron distributions in the Yb nucleus.

D. Antypas, A. Fabricant, V. V. Flambaum, J.E. Stalnaker, K. Tsigutkin, and D. Budker, Nature Physics 15, 120 (2019)

Nuclear spin-dependent

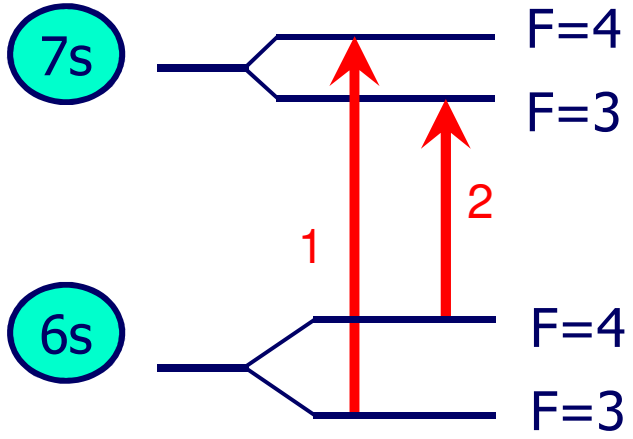
parity violation effects

Parity violation in atoms: weak interactions inside the nuclei



Parity-violating nuclear moment

Valence nucleon density



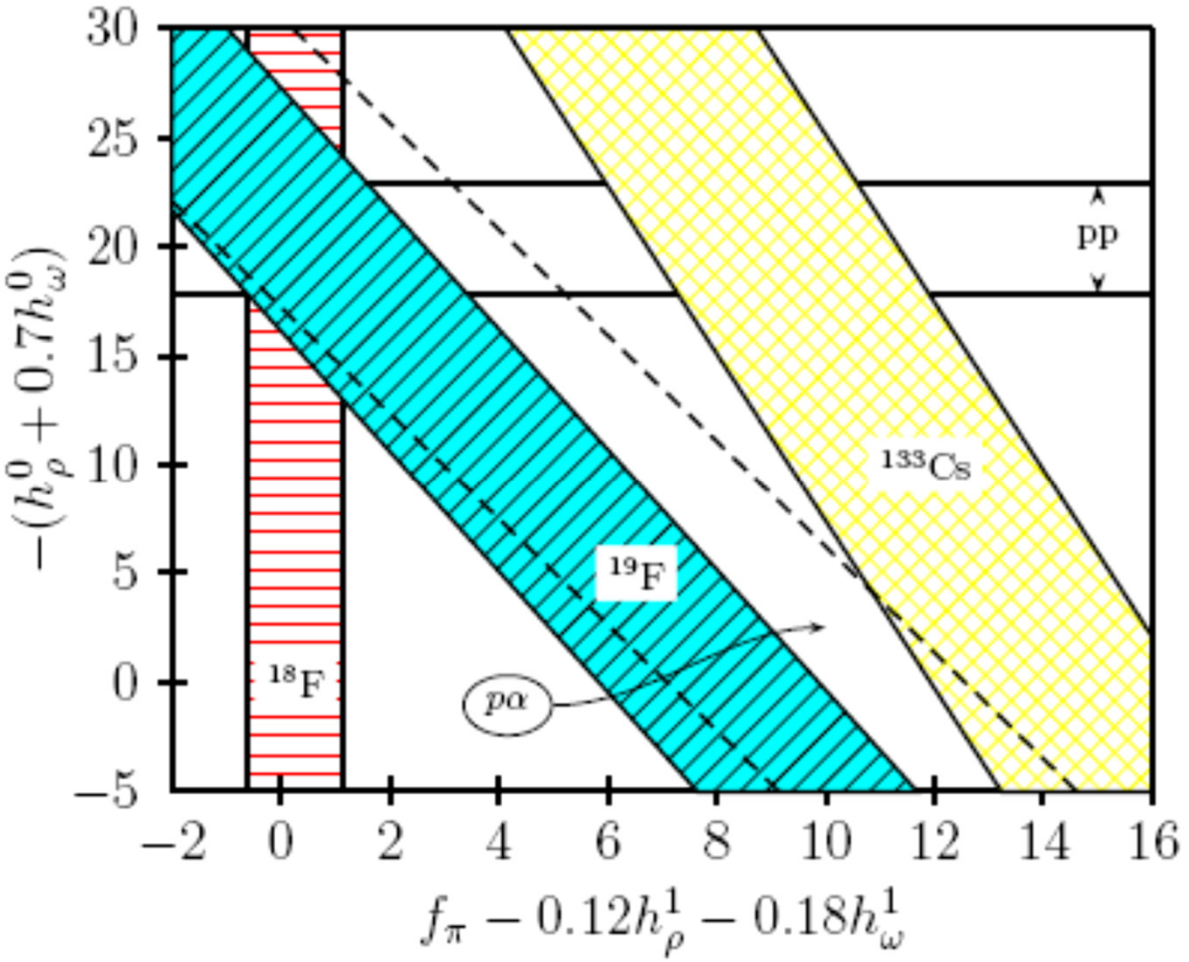
$$H^{(a)}_{PNC} = \frac{G_F}{\sqrt{2}} \kappa_a \, \boldsymbol{\alpha} \cdot \mathbf{I} \; \rho_v(r)$$

Anapole moment

Need theory to extract anapole moment from experiment

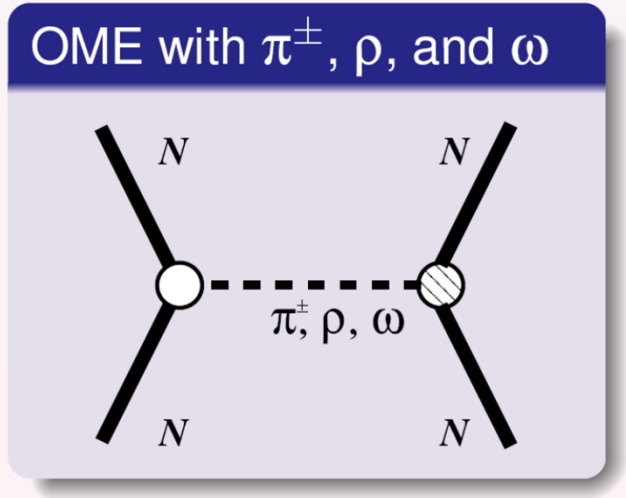
Nuclear anapole moment is parity-odd, time-reversal-even E1 moment of the electromagnetic current operator.

Constraints on nuclear weak coupling constants: Cs parity violation diasgrees with nuclear experiments



Meson exchange picture

Building blocks: nucleon, mesons, and their couplings



From: Cheng-Pang Liu

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

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:

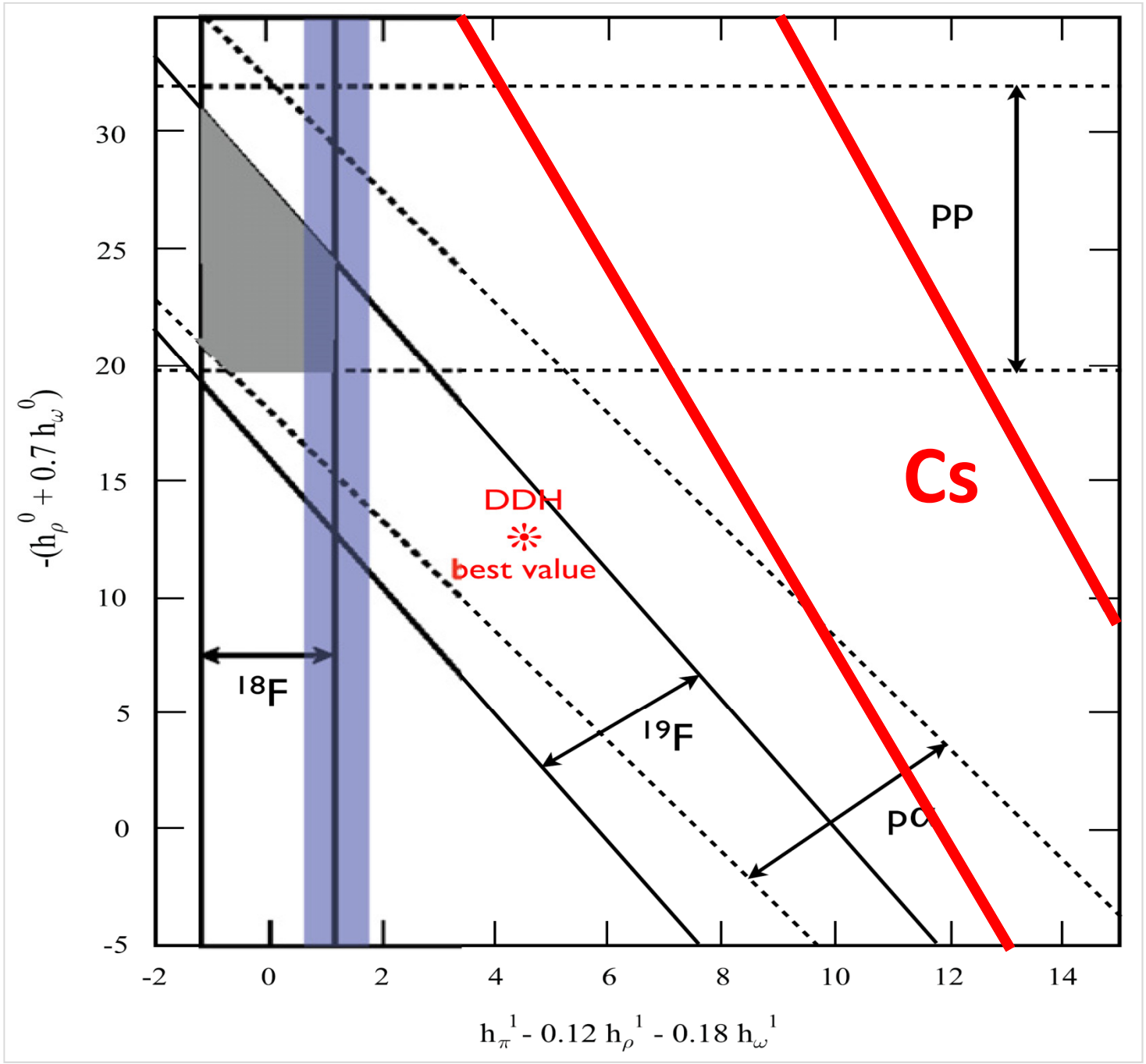
$k = 0.107(16)$ [better than 5% theory accuracy]

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

Need new experiments

Cs, Fr, Yb, Ra^+, molecules

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



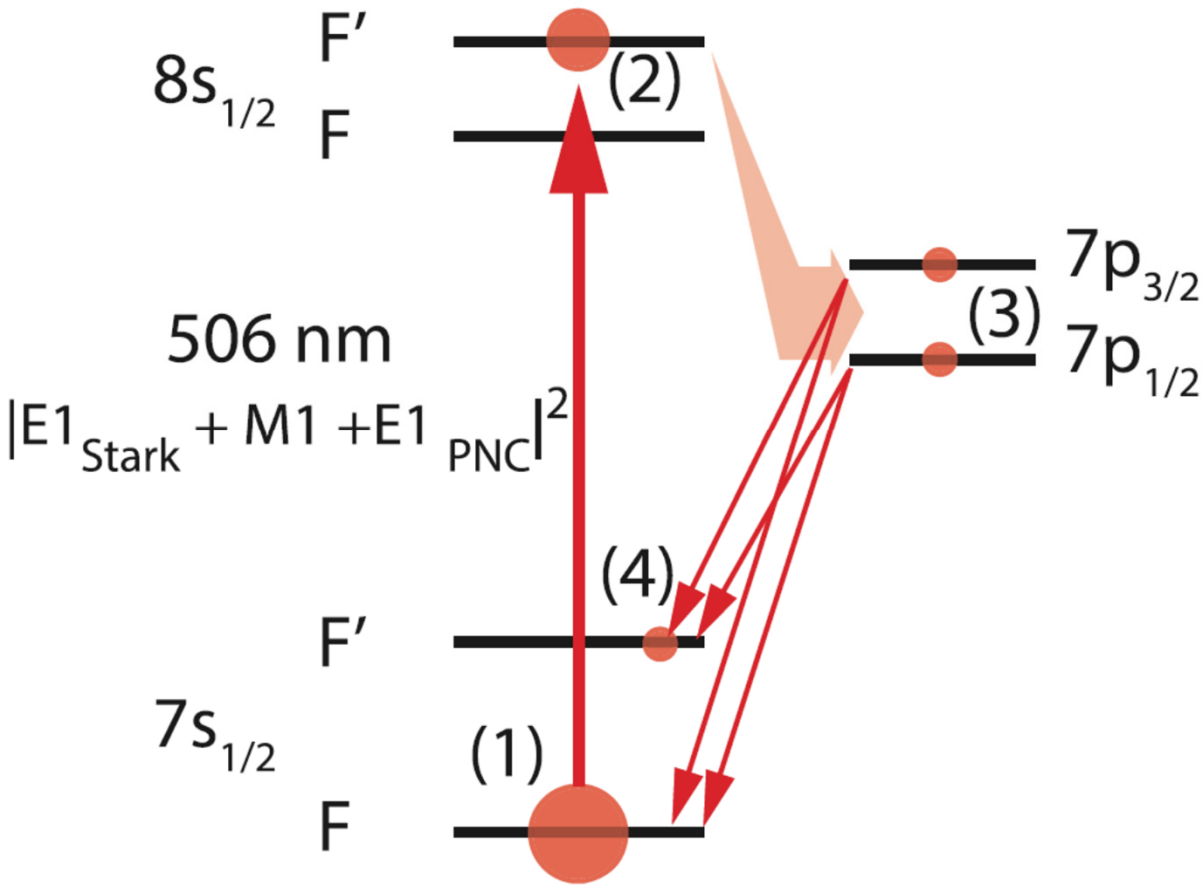
Cs extraction of anapole moment atomic theory accuracy
better than 5%
Expt.: 15%

W.C. Haxton and B.R. Holstein, Progress in Particle and Nuclear Physics 71, 185 (2013)

Towards measurements of atomic parity non-conservation in francium

Fr: both 7s hyperfine and 7s-8s experiments

TRIUMF



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Projected constraints of couplings from measuring two francium isotopes

TRIUMF

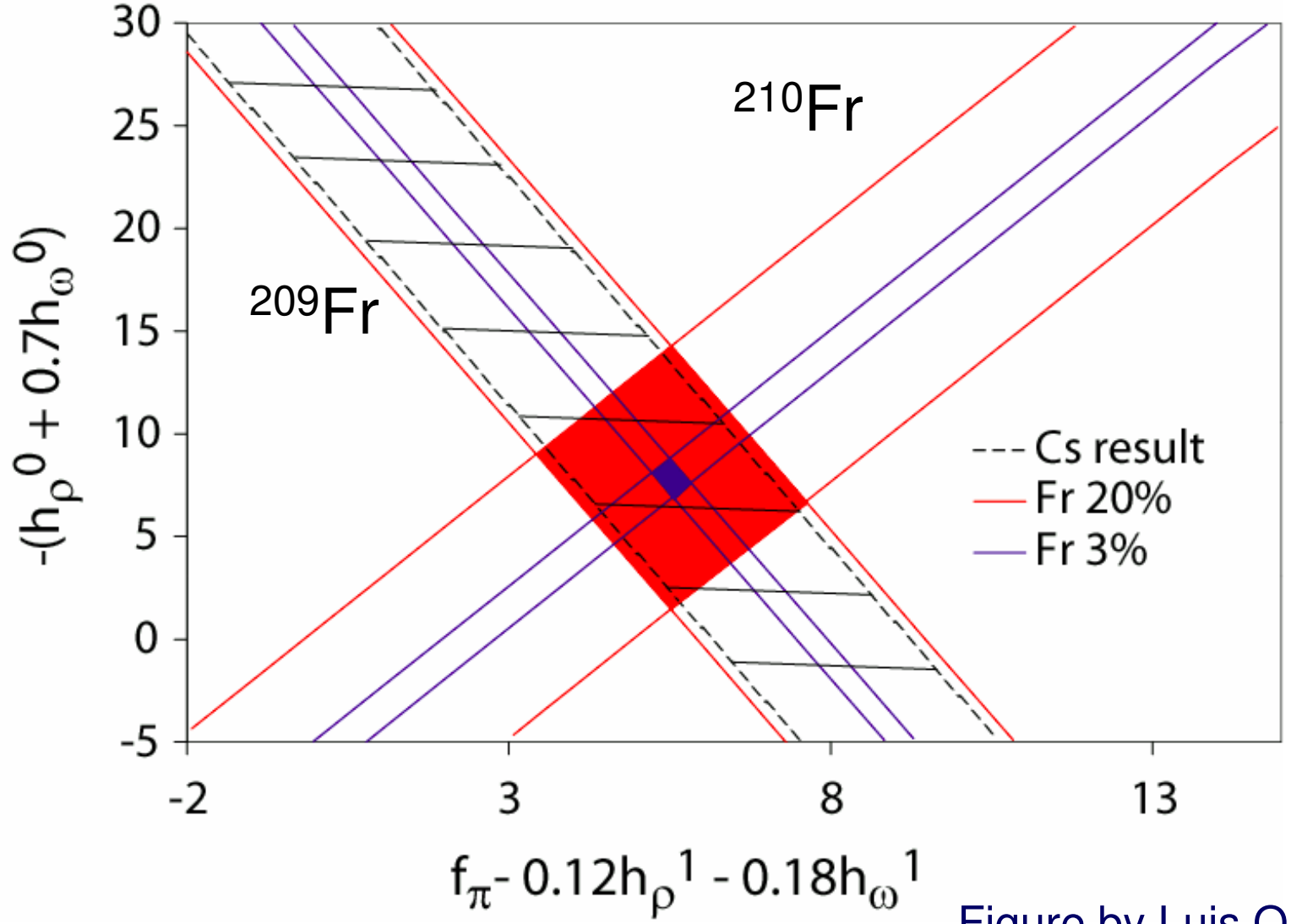


Figure by Luis Orozco

Other APV measurements

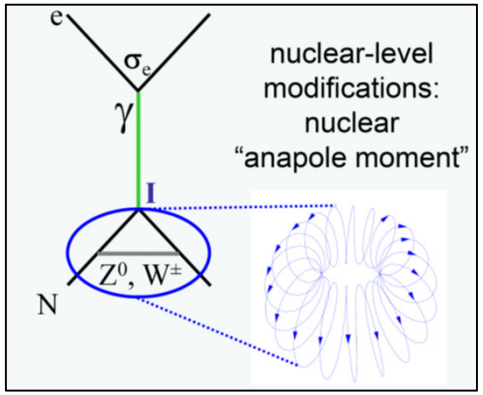
Cs at Purdue

Measurement of the lifetimes of the and states of atomic cesium G Toh, et al. Physical Review A 100 (5), 052507 (2019)

Determination of the Scalar and Vector Polarizabilities of the Cesium Transition and Implications for Atomic Parity Nonconservation, G Toh, A Damitz, CE Tanner, WR Johnson, DS Elliott, Physical Review Letters 123, 073002 (2019)

Ra^+ at UCSB (Laser cooled and trapped)

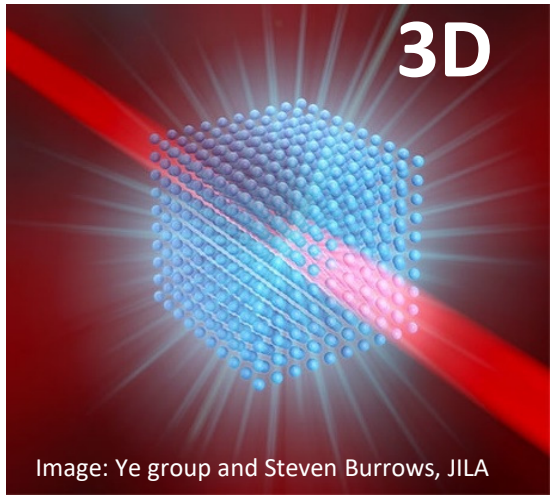
C. A. Holliman, M. Fan, A. Contractor, S. M. Brewer, A. M. Jayich, PRL 128, 033202 (2020)



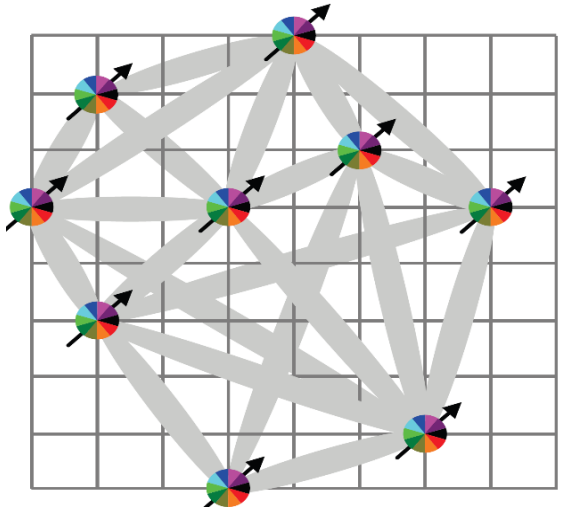
ZOMBIES: Measuring strong-force induced modifications of electroweak interactions (molecules) Dave DeMille's group

Recent Developments in Atomic theory for fundamental physics and other applications

Numerous applications that need precise atomic data

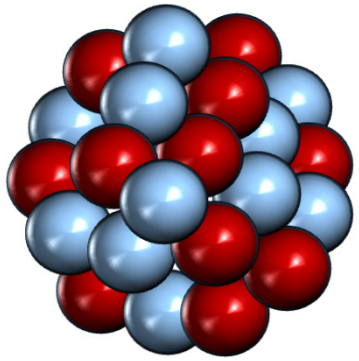


Atomic clocks



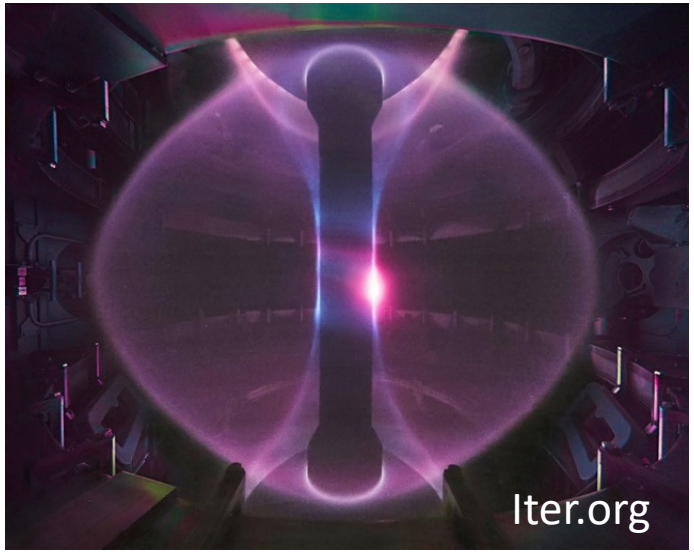
Ultracold atoms
Quantum simulation

Particle physics:
Searches for dark matter and other
"new" physics



Nuclear and hadronic physics -
extracting nuclear properties

Astrophysics



Plasma physics

Development of new methods for high-precision atomic calculations

Method and code developers:

Charles Cheung (University of Delaware, USA)
Sergey Porsev (University of Delaware, USA, PNPI, Russia)
Mikhail Kozlov (PNPI, Russia)
Ilya Tupitsyn (University of St. Petersburg, Russia)
Andrey Bondarev, (St. Petersburg Polytechnic University, Russia
Marianna Safronova (University of Delaware, USA)

Methods:

Coupled-cluster (all-order) LCCSD, CCSDvT, CCSDT (new), new OpenMP codes
Configuration interaction CI (new MPI CI code)
Configuration interaction + valence PT (MPI CI+PT code)
Hybrid configuration interaction and coupled-cluster approaches:
CI+MBPT and CI+all-order (CI+LCCSD and new CI+CCSDvT)

L: linearized
CC: coupled-cluster
S: single excitations
D: double excitations
T: triple excitations
vT: valence triple excitations
PT: perturbation theory
MPI: message passing interface

Capabilities:

(1) accurate calculations of a very wide range of atomic properties for atoms and positive and negative ions with a few valence electrons (currently tested up to 6 valence electrons)

(2) new capabilities to calculate more complicated systems with MPI CI and MPI CI+PT

Intrinsically relativistic, QED (can choose among 4 potentials) and full Breit interaction is included

Development of new methods for high-precision atomic calculations

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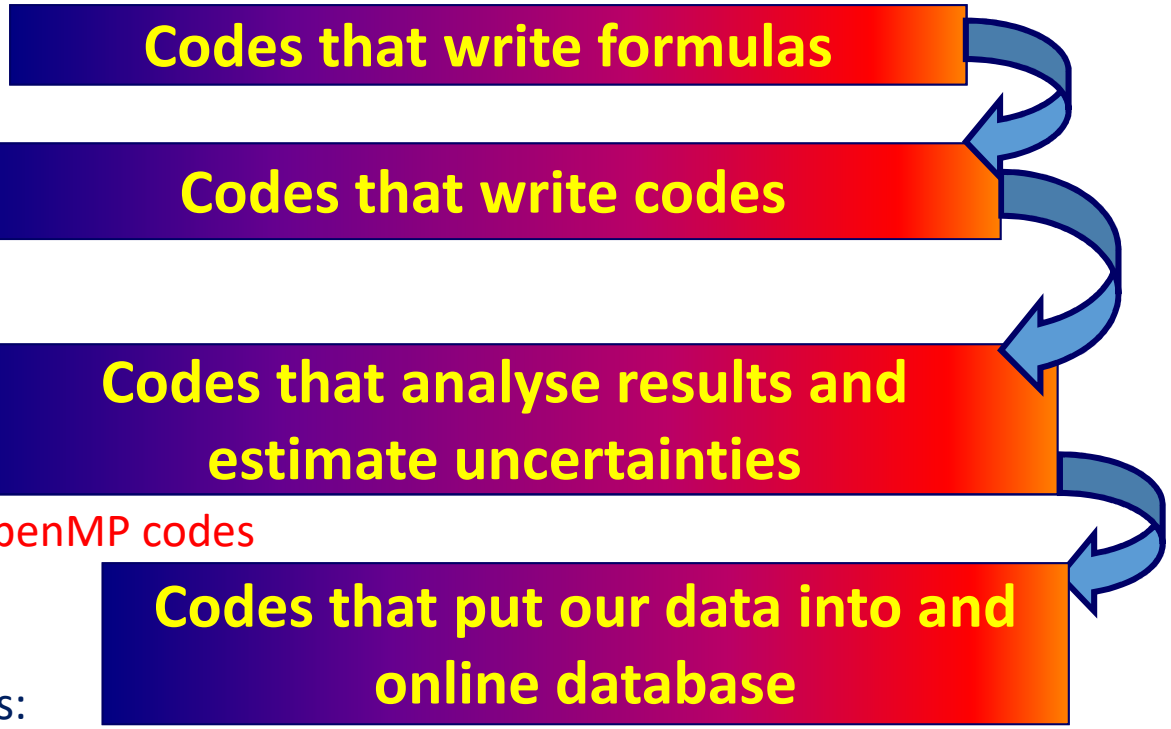

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Coupled-cluster (all-order) LCCSD, CCSDvT, CCSDT (new), new OpenMP codes
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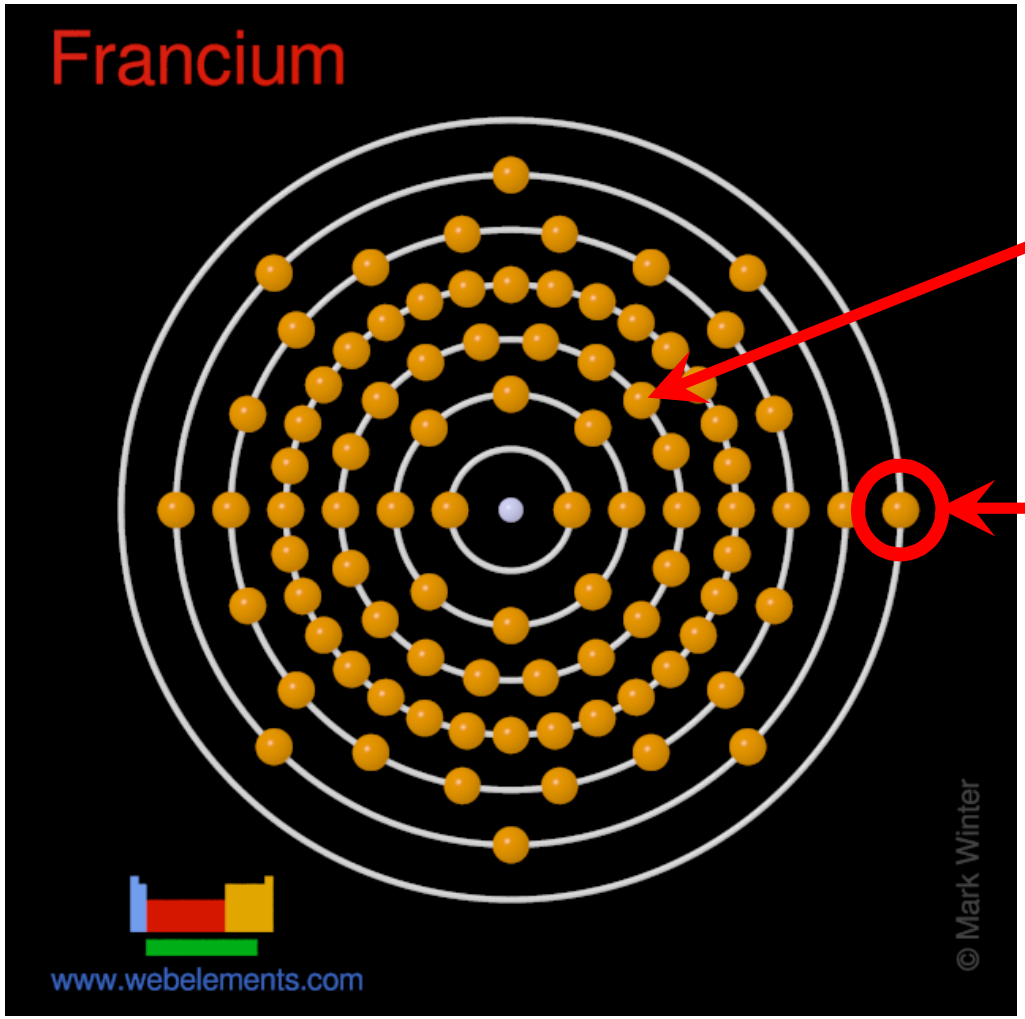
Atomic calculations: closed shells vs. valence electrons

Atomic physics can use a “mean field” – nucleus + inner electrons.

If the number of “valence electrons” is small computations can be done with high precision.



Closed shells

Can be approximated by a mean field

Single valence electron

7s for Fr

5f for Th^{3+}

Code and method development I

Development of full CCSDT relativistic coupled cluster method

First inclusion of core triples!

Example: Th^{3+}

PHYSICAL REVIEW A **88**, 060501(R) (2013)

LCCSDpT level + fit

Magnetic dipole and electric quadrupole moments of the ^{229}Th nucleus

M. S. Safronova,[1,2] U. I. Safronova,[3,4] A. G. Radnaev,[5,6] C. J. Campbell,[6] and A. Kuzmich[6]

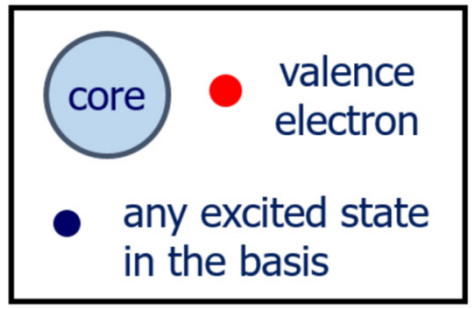
- We determined the magnetic dipole **μ = 0.360(7) μ_N** and the electric quadrupole Q = 3.11(6) eb moments of the ^{229}Th nucleus.

- We find that the previous value **μ = 0.46(4) μ_N** [Gerstenkorn *et al.*, J. Phys. (Paris) **35**, 483 (1974)] is incorrect by 25%.

- We report a method for determining the accuracy of theoretical hyperfine constants B/Q and demonstrate that it can be used to extract the electric quadrupole moment ***Q* with a 1%–2% uncertainty** for a large number of nuclei.

- This approach allowed us to identify 40% inconsistencies in measurements of Ra^+ hyperfine constants B.

Coupled-cluster method (CCSDvT)



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

⇓

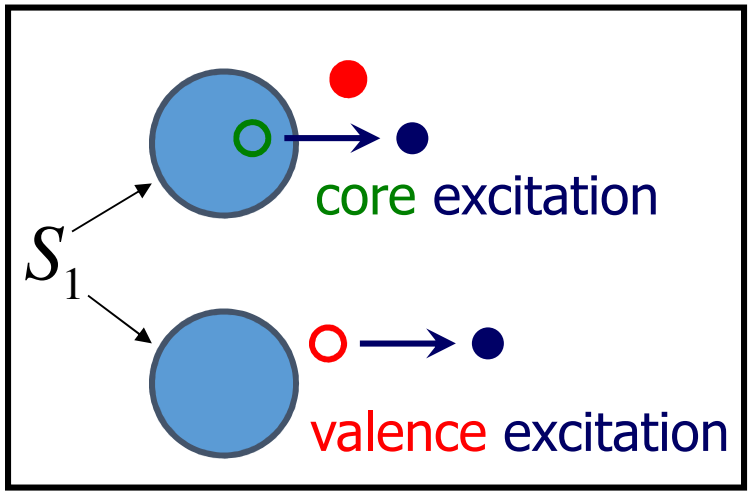
$\exp(S_1 + S_2 + S_3)$ **CCSDT single-double-triple coupled-cluster**

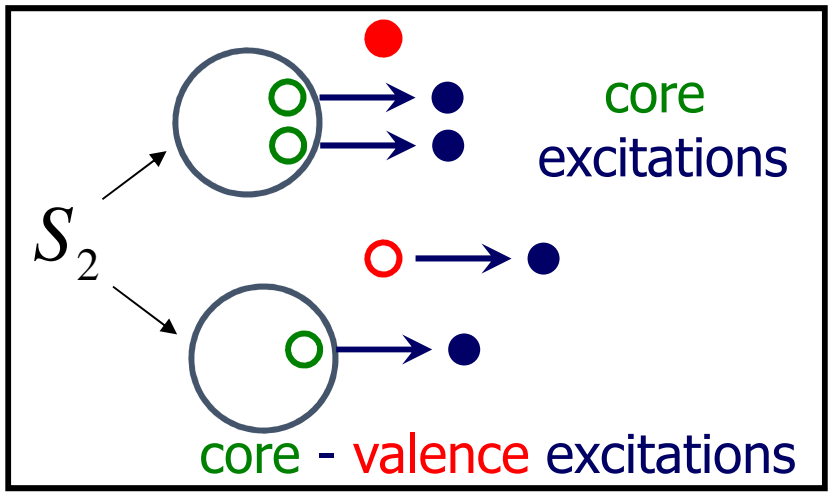
$\exp(S_1 + S_2 + S_{v3})$ **single-double- valence triple**

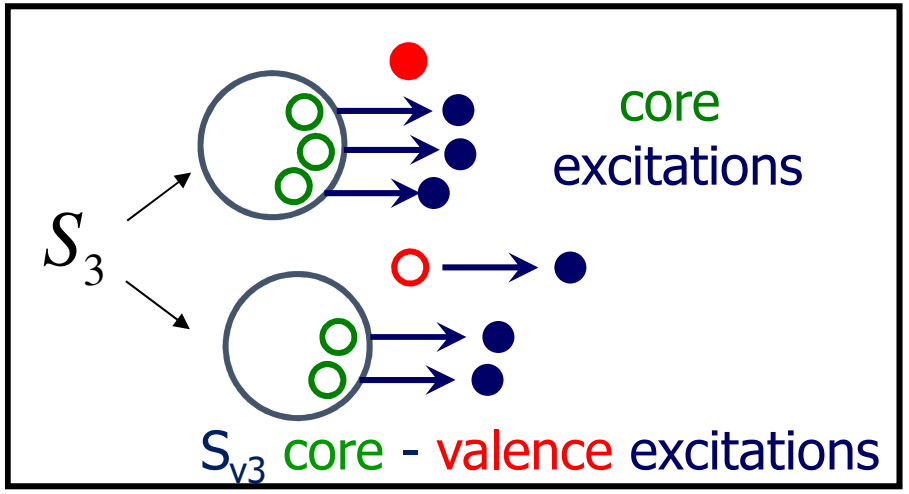
⇓

$S_1 + S_2 + S_{v3}$ **LCCSDvT coupled-cluster**

ALL excitations (300-1000 orbitals)







Nonlinear terms: $S_1^2, S_2^2, S_1S_2, \ldots$

New work:

CCSDT with core triples is now fully implemented (OpenMP)

valence triples accelerated by a factor of 10

Energies of Th^{3+}: comparing various version of CC method

TABLE I. The removal energies of the $5f_{5/2;7/2}$ and $6d_{3/2;5/2}$ states for Th^{3+} (in cm^{-1}) in different approximations, discussed in the text, are presented. The theoretical total and experimental results are given in the rows E_{total} and E_{expt}. The difference between the total and experimental values is presented (in %) in the row labeled "Diff. (%)".

	$5f_{5/2}$	$5f_{7/2}$	$6d_{3/2}$	$6d_{5/2}$
E_{BDHF}	207310	203393	211842	207686
E_{LCCSD}	232308	227978	222871	217543
E_{CCSDT}	231640	227307	222490	217174
E_{CCSDvT}	230819	226538	222472	217259
E_{CCSDT}	230693	226398	222268	217032
ΔE_{extrap}	1055	1032	257	242
E_{total}	231748	227431	222526	217274
E_{expt} [20, 21]	231065	226740	221872	216579
Diff. (%)	0.30	0.30	0.29	0.32
Δ_{LCCSD} [a]	2298	2271	1256	1205
Δ_{CCSD} [b]	1630	1599	875	836
Δ_{CCSDvT} [c]	809	831	857	922
Δ_{CCSDT} [d]	683	691	654	695

[a] $\Delta_{LCCSD} \equiv E_{LCCSD} + \Delta E_{extrap} - E_{expt}$;
[b] $\Delta_{CCSD} \equiv E_{CCSD} + \Delta E_{extrap} - E_{expt}$;
[c] $\Delta_{CCSDvT} \equiv E_{CCSDvT} + \Delta E_{extrap} - E_{expt}$;
[d] $\Delta_{CCSDT} \equiv E_{CCSDT} + \Delta E_{extrap} - E_{expt}$.

First inclusion of core triples!

TABLE II. The theoretical and experimental [21] transition energies of the excited states counted from the ground state.

	Theory	Experiment	Diff.	Diff %
$5f_{5/2}$	0	0		
$5f_{7/2}$	4318	4325	7	0.16%
$6d_{3/2}$	9223	9193	-30	-0.33%
$6d_{5/2}$	14475	14486	11	0.08%

S. G. Porsev, M. S. Safronova, and M. G. Kozlov, Phys. Rev. Lett. 127, 253001 (2021).

Hyperfine constant A and extracting ^{229}Th nuclear magnetic dipole moment

$$A_t \equiv A/g \text{ (where } g = (\mu/\mu_N)/I$$

TABLE III. Different contributions to A_t (in MHz) and obtaining the recommended value of g are explained in the text. The experimental values of the HFS constants A [23] are given in the row labeled "A(experim.)". The uncertainties are given in parentheses.

	$5f_{5/2}$	$5f_{7/2}$	$6d_{3/2}$	$6d_{5/2}$
BDHF	507	263	831	304
Δ(SD)	72	-45	268	-386
LCCSD	579	218	1099	-81
Δ(NL)	-3.3	-4.6	-17	18
Δ(vT)	-12	-5.1	-21	-46
Δ(cT)	-1.5	-2.3	5.8	-1.8
CCSDT	562	206	1067	-111
Basis extrap.	-0.2	2.6	-4.5	7.1
Total	562(3)	209(3)	1063(12)	-104(22)
Ref. [6][a]	573	215	1079	-92
A(experim.) [23]	82.2(6)	31.4(7)	155.3(1.2)	-12.6(7)

S. G. Porsev, M. S. Safronova, and M. G. Kozlov, Phys. Rev. Lett. 127, 253001 (2021).

Bohr–Weisskopf effect

A real nuclear magnetization can differ from the uniform magnetization.

Yu. A. Demidov et al., Phys. Rev. A 103, 032824 (2021).

$$A = g\,A_0\,(1 - d_{\text{nuc}}\,y)$$

A_0 is the theoretical value calculated at the point-like magnetization of the nucleus

d_{nuc} and y are the parameters depending on the nuclear and electronic structure, respectively

Calculate $y = 1 - A_t/A_0$

$$g \approx 0.1465(24)$$
$$d_{\text{nuc}} \approx 1.7(2.1)$$
$$\mu = gI \approx 0.366(6)\mu_N$$

Need realistic magnetization distribution and more precision hyperfine measurements!

Hyperfine constant B and extracting ^{229}Th nuclear electric quadrupole moment

Different contributions to the electric quadrupole hypefine constants *B/Q* (in MHz/(eb)) for $^{229}Th^{3+}$

	$5f_{5/2}$	$5f_{7/2}$	$6d_{3/2}$	$6d_{5/2}$
BDHF	535	572	611	648
Δ(SD)	202	251	132	228
LCCSD	737	822	743	877
Δ(NL)	38	45	9	9
Δ(vT)	-55	-57	-34	-27
Δ(cT)	3	3	7	7
CCSDT	723	814	725	866
Basis extrap.	6	8	3	4
Total	729(10)	822(13)	728(6)	869(11)
Ref. [6]	725	809	738	873
Ref. [22]	740	860	690	860
B(experim.) [23]	2269(2)	2550(12)	2265(9)	2694(7)
Q	3.11(4)	3.10(5)	3.11(3)	3.10(4)
Q(recommended)		3.11(2)		
Ref. [6]		3.11(6)		
Refs. [22, 23]		3.11(16)[a]		

More valence electrons: 2 to 6

Code and method development II

Combining configuration interaction and coupled cluster method

---

First tests for 6 valence electrons

Examples: Ac, No, Th+, Th^{2+}, U^{+} and U

Configuration interaction

Use **configuration interaction** (CI) method to treat valence correlations

$$\Psi = \sum_i c_i \Phi_i$$

Number of configurations blows up exponentially with the number of valence electrons!

150 orbitals in the basis set

$$150^2 = 22\,500$$

$$150^4 = 506\,250\,000$$

$$150^6 = 11\,390\,625\,000\,000$$

Good news: only a small subset of these configuration needs to be included, but which ones?

Electron-electron correlation separates into two problems

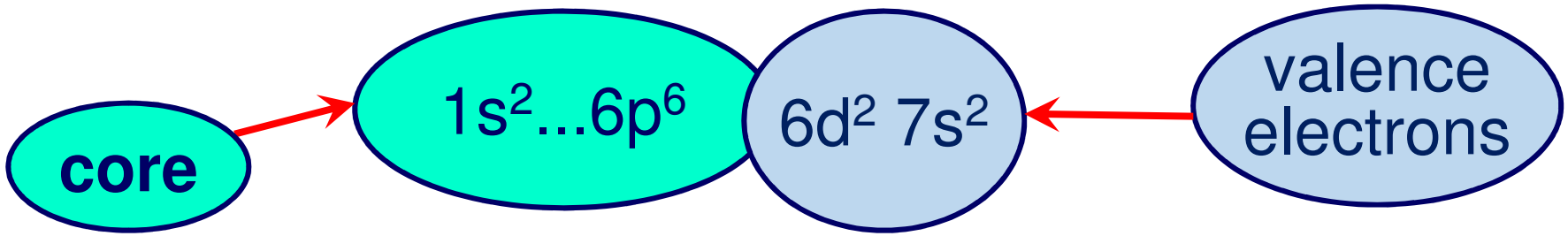
Orbital angular momentum l

s	$l=0$
p	$l=1$
d	$l=2$
f	$l=3$

Example: Thorium Z = 90

Four valence electrons outside of a closed core

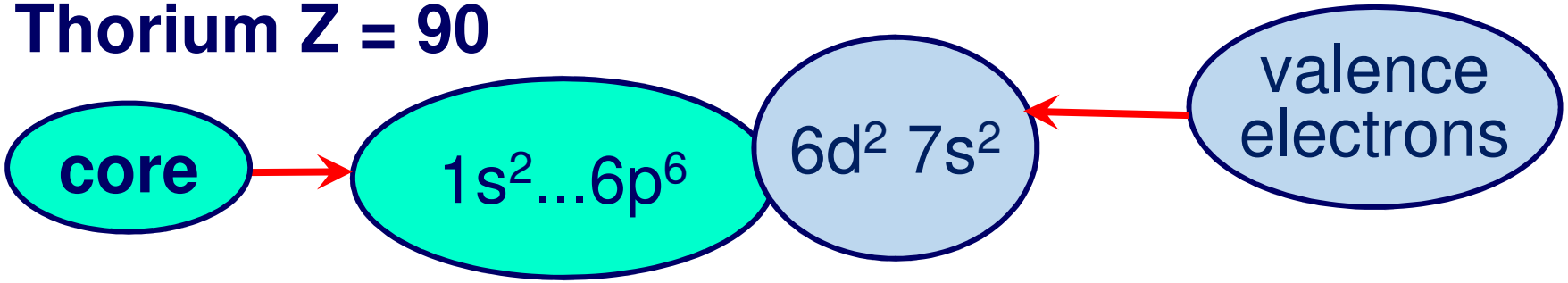
$[1s^2 \ldots 4f^{14}5d^{10}6s^26p^6]\ 6d^2\ 7s^2\ {}^3F_2$ ground state



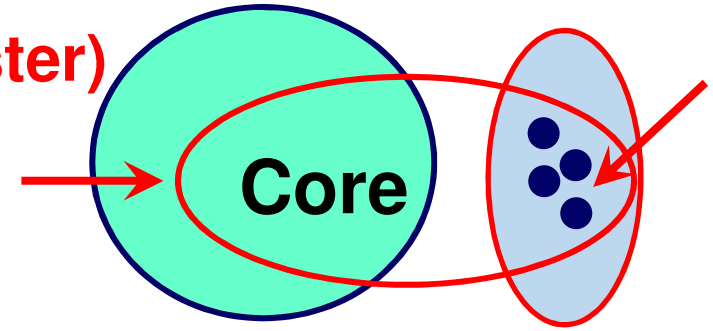
Problem 1: core-core and core-valence correlations

Problem 2: valence-valence correlations

Electron-electron correlation separates into two problems



Use all-order **(coupled-cluster)** method to treat core and core-valence correlations



Use **configuration interaction** (CI) method to treat valence correlations

$$H_1^{eff} = H_1 + \Sigma_1$$

$$H_2^{eff} = H_2 + \Sigma_2$$

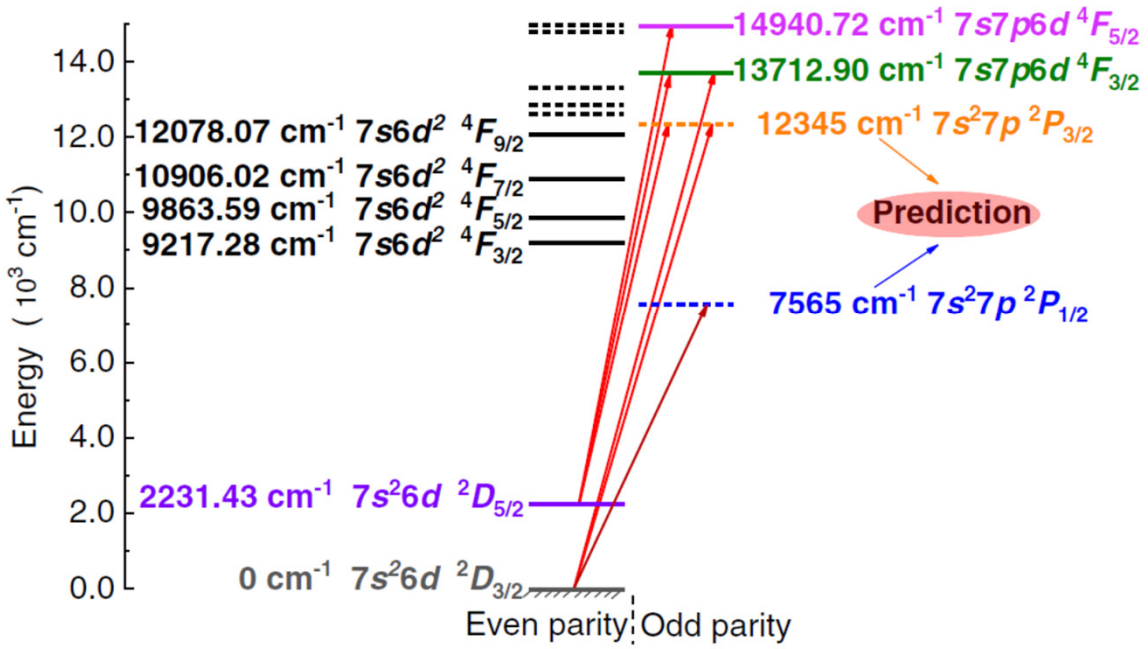
valence

$$\Psi = \sum_i c_i \Phi_i$$

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

Detection of missing low-lying atomic states in actinium

K. Zhang et al., Phys. Rev. Lett. 125, 073001 (2020)



State		Energy (cm^{-1}) Experiment	Calculation
$7s^27p$	$^2P^o_{1/2}$	7477.36(4)	7701(250)
$7s^27p$	$^2P^o_{3/2}$	12276.59(2)	12475(250)
$7s7p6d$	$^4F^o_{3/2}$	13712.74(3)	13994(370)

State		$\tau(ns)$ Experiment	Calculation I	Calculation II
$7s^27p$	$^2P^o_{1/2}$	668(11)	647	707(53)
$7s^27p$	$^2P^o_{3/2}$	255(7)	209	219(16)
$7s7p6d$	$^4F^o_{3/2}$	352(11)	327	351(29)

PHYSICAL REVIEW LETTERS **121,** 213001 (2018)

Nuclear Charge Radii of ^{229}Th from Isotope and Isomer Shifts

M. S. Safronova,[1,2] S. G. Porsev,[1,3] M. G. Kozlov,[3,4] J. Thielking,[5] M. V. Okhapkin,[5]
P. Głowacki,[5,*] D. M. Meier,[5] and E. Peik[5]

We carried out isotope shift calculations in Th^{+} and Th^{2+}.

Combined with experimental measurements of PTB for isotopic shift between $^{229}Th^{2+}$ and $^{232}Th^{2+}$ to extract : $^{+}$

$$\delta\langle r^2\rangle^{232,229} = 0.299(15)\ \text{fm}^2$$

Previous value: 0.33(5) fm².

Using the recently measured values of the isomer shift of lines of ^{229m}Th, we derive the value for the mean-square radius change between ^{229}Th and its low-lying isomer ^{229m}Th to be

$$\delta\langle r^2\rangle^{229m,229} = 0.0105(13)\ \text{fm}^2$$

Extraction of No nuclear properties from laser spectroscopy

$$A_{\mathrm{HFS}} = \mu(B_e/IJ) \qquad B_{\mathrm{HFS}} = eQ_s\langle(\partial^2 V/\partial z^2)\rangle$$

	Hyperfine splitting for ^{253}No		Isotope shift
Atomic calculations	B_e/J (GHz $\cdot I/\mu_N$)	$\langle\partial^2 V/\partial z^2\rangle$ (GHz/eb)	F_s (GHz/fm^2)
CI + all orders	−6.3(0.9)[a]	0.486(70)[a]	−95.8(7.0)[a]
CI + MBPT	−7.1(1.0)	0.503(75)	−104(10)
CIPT	−7.4(1.2)	0.624(90)	−94(25)
FSCC		0.465(70)[a]	−99(15)
MCDF	−4.1(1.8)	0.444(75)	−113(25)
Spectroscopic results	A_{HFS} (GHz)	B_{HFS} (GHz)	$\delta\nu^{254,253}$ (GHz)
	0.734(46)	2.82(69)	6.72(18)
Nuclear properties	$\mu(\mu_N)$	Q_s (eb)	$\delta\langle r^2\rangle^{254,253}$ (fm^2)
	−0.527(33)(75)	+5.9(1.4)(0.9)	−0.070(2)(5)

Probing sizes and shapes of nobelium isotopes by laser spectroscopy,
S. Raeder et al., Phys. Rev. Lett. 120, 232503 (2018)

Energy levels of U^+ and U

TABLE I. The energies of the excited states (in cm^{-1}), counted from the ground state, calculated in the CI+MBPT and CI+all-order approximations. The CI+all-order values are presented for different sets of the configurations. The QED corrections are given in the column labeled "QED". The final values, given in the column labeled "Final", are found as the sum of the CI+all-order values obtained for $[21spdf13g]$ and the QED corrections. The experimental values are given in the last two columns.

	Level	CI+MBPT	CI+all-order				Final	Experiment	
		$[13spdfg]$	$[13spdfg]$	$[15spdf13g]$	$[17spdf13g]$	$[21spdf13g]$	QED		Ref. [4]	Ref. [5]
U^+	$5f^3 7s^2\ {}^4I_{9/2}$	0	0	0	0	0	0	0	0	
	$5f^3 6d7s\ {}^6L_{11/2}$	1411	497	498	409	450	-175	274	289	
	$5f^3 6d7s\ {}^6K_{9/2}$	1896	1088	1088	1003	1033	-170	862	915	
	$5f^3 6d7s\ {}^6L_{13/2}$	3008	2006	2005	1907	1934	-188	1746	1749	
	$5f^3 6d7s\ {}^6K_{11/2}$	3382	2471	2470	2377	2396	-180	2215	2295	
U	$5f^3 6d7s^2\ {}^5L_6$	0	0	0	0	0	0	0		0
	$5f^3 6d7s^2\ {}^5L_7$	4420	3772	3779	3775	3784	8	3792		3801
	$5f^3 6d7s^2\ {}^5K_6$	4757	4221	4231	4225	4225	10	4235		4276

Test of CI+LCCSD for 6 valence electrons!

Calculation of energies and hyperfine structure constants of $^{233}U^+$ and ^{233}U,
S. G. Porsev, C. Cheung, M. S. Safronova, arXiv:2204.13214 (2022)

151,000,000 determinants
1600 CPUs
24.2 TB memory!

Even more valence electrons

Code and method development III
Configuration interaction

New fast MPI code
broadly applicable

Example: Th^{35+}

Performance test of the parallel code

From 2 weeks to 15 minutes!

Ir^{17+} , 52 basis functions, 30 valence e^-, 25K conf-s, 17.4M det-s, 27.7B matrix elements

Serial code: 2 weeks of runtime

Number		Memory	Time (seconds)			Speedup		
nodes	cores	per core	Construct	Solve	Total	Construct	Solve	Total
1	64	9.1GB	4h 32m	28m 56s	5h 3m	1	1	1
2	128	5.5GB	2h 15m	16m 27s	2h 32m	2.02	1.76	1.98
4	256	3.7GB	1h 7m	9m 57s	1h 18m	4.05	2.91	3.84
8	512	2.8GB	33m 27s	6m 18s	41m 31s	8.13	4.59	7.30
16	1024	2.4GB	16m 41s	4m 33s	23m 3s	16.29	6.36	13.14
32	2048	2.1GB	8m 21s	4m 2s	**14m 57s**	32.55	7.17	20.26

A PATHWAY TO EXCITE A NUCLEAR TRANSITION: ELECTRONIC BRIDGE IN Th^{35+}

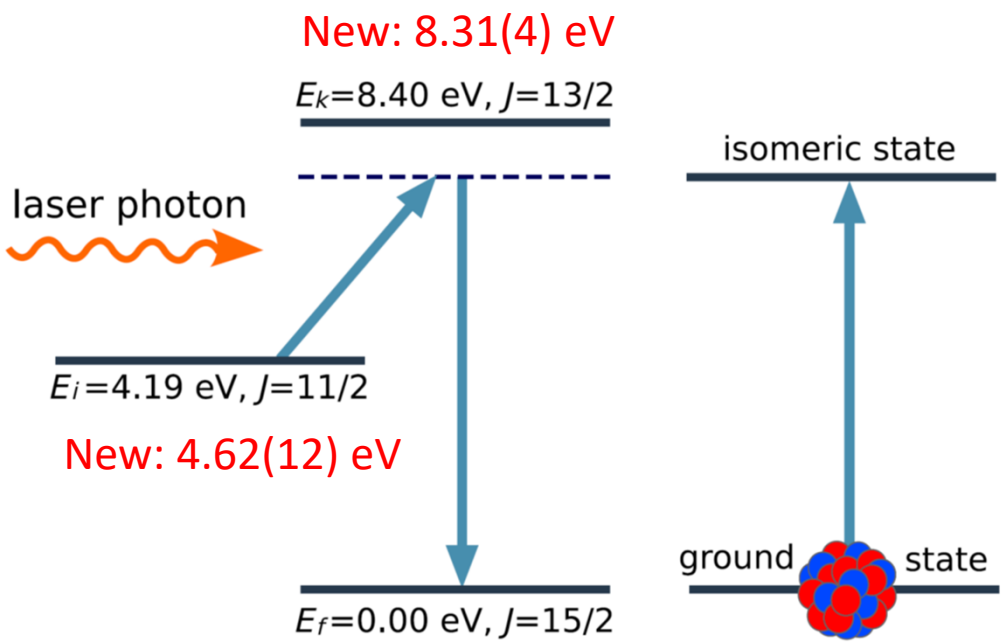


Figure: Bilous et al., Phys. Rev. Lett. 124, 192502 (2020)

Low-lying energy levels of $^{229}Th^{35+}$ and the electronic bridge process, S. G. Porsev, C. Cheung, M. S. Safronova, Quantum Sci. Technol. 6, 034014 (2021)

TABLE II. The energies obtained in the framework of 9-, 19-, and 25-electron CI calculations with the excitations allowed to $[7spdfgh]$, are presented. The main configurations of the valence electrons are given in the first column. The energies of the excited states, counted from the ground state energy, are given in the columns labeled "E" (in cm^{-1}). The differences $E(4d^{10}4f^9) - E(4f^9)$ and $E(4p^64d^{10}4f^9) - E(4d^{10}4f^9)$ are given for each state in the column labeled "Δ" in cm^{-1}. The sum $\Delta(4d^{10}4f^9) + \Delta(4p^64d^{10}4f^9)$ is presented in the row labeled "Total".

	$J=11/2$		$J=13/2$	
	E	Δ	E	Δ
$4f^9$	36411		67255	
$4d^{10}4f^9$	37400	989	66948	-307
$4p^64d^{10}4f^9$	37487	87	66899	-49
Total		1076		-356

$$E_{J=13/2} \approx 67000\,(315)\ \mathrm{cm}^{-1} \approx 8.307(39)\ \mathrm{eV}$$

New MPI code, 120 million determinants, code tests to 1500 CPUs!

Next step: selection of configurations with neural networks

COMPUTER, CALCULATE!

Automating all codes for massive data generation

Turn research codes into software!

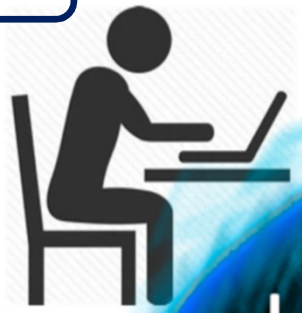
Community – driven project: there is enormous need for data

https://www.udel.edu/atom

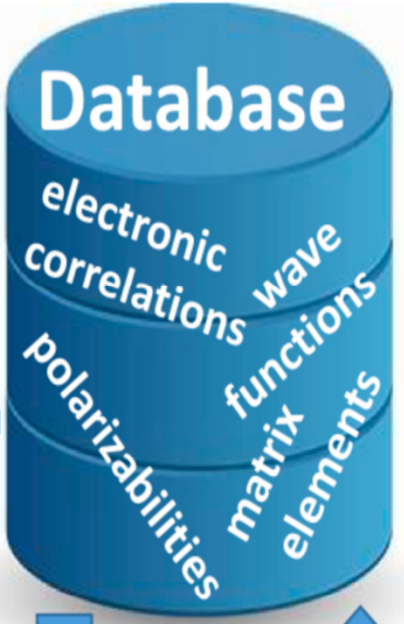
Version 2 was released on April 2022

Applications in science and engineering

- quantum information
- degenerate quantum gases
- atomic clocks
- precision measurements
- plasma physics
- astrophysics
- studies of fundamental physics



High-Precision Atomic Physics Portal



on-demand execution

automatic ingest

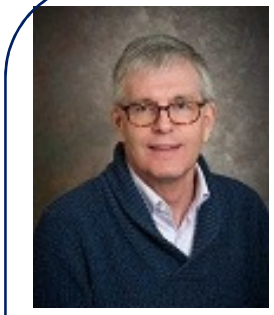
Atomic Physics computational codes

Building on:

- CI+MBPT/CI+all-order program package and expertise
- Portal technology (Science Gateways, Hubzero,…)
- Parallel programming methodology

UD team and collaborators

Online portal team



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