UNSW
THE UNIVERSITY OF NEW SOUTH WALES

Neutron skin and parity-violating transitions in atoms

V. A. Dzuba and V. V. Flambaum

University of New South Wales, Sydney, Australia

Two questions:

- Can the measurements of parity-violating transitions can be used to study neutron skin?
- To what extend neutron skin uncertainty affects the search for new physics beyond SM?

Two types of measurements:

- Single-isotope measurement of PV violating transition in atom (e.g. the 6s-7s transition in Cs).
- The ratio of PV violating amplitudes for two isotopes.

Follow the works:

A. Derevianko, and S. G. Porsev, PRA **65**, 052115 (2002);
B. A. Brown, A. Derevianko, and V. V. Flambaum, PRC **79**, 035501 (2009);
V. A. Dzuba, numerical analysis (unpublished, 2016).

Single-isotope PV amplitude

$$\frac{\Delta E_{PV}^{NS}}{E_{PV}} = K\frac{\Delta R_{np}}{R_p} \qquad K \approx -\frac{3}{7}(\alpha Z)^2$$

$$\frac{E_{\text{expt}} - E_{\text{theor}}^{0}}{E_{\text{theor}}^{0}} = K\frac{\Delta R_{np}}{R_p} \qquad E_{\text{theor}}^{0} \text{ calculated at } R_n = R_p$$

Atom	K	$-(3/7)(\alpha Z)^2$	$K\Delta R_{np}/R_p$
^{133}Cs	-0.0769	-0.0691	-0.0026(5)
^{138}Ba	-0.0797	-0.0716	-0.0030(6)
^{221}Fr	-0.1881	-0.1727	-0.0070(16)
^{222}Ra	-0.2010	-0.1841	-0.0068(16)

$\Delta R_{np}/R_p$: Brown, Derevianko, Flambaum, PRC **79**, 035502 (2009);

High accuracy is needed for both E_{expt} and E_{theor}^{0}

The highest accuracy has been achieved for cesium

Experiment:

$$-\mathrm{Im}(E_{PV})/\beta = 1.5935(1 \pm 0.35\%)\mathrm{mV/cm}$$ Boulder, 1997

Theory is good for alkali atoms (Cs, Fr, etc.), e.g., for Cs:

Epv	Source
0.88(3)	Dzuba, Flambaum, Silvestrov, Sushkov (1984)
0.90(2)	Dzuba, Flambaum, Silvestrov, Sushkov (1987)
0.95(5)	Johnson, Blundell, Liu, Sapirstein (1988)
0.908(9)	Dzuba, Flambaum, Sushkov (1989)
0.909(9)	Blundell, Johnson, Sapirstein (1990)
0.905(9)	Kozlov, Porsev, Tupitsin (2001)
0.9078(45)	Dzuba, Flambaum, Ginges (2002)
0.8990(24)*	Porsev, Derevianko, Beloy (2009)
0.9079(40)#	Dzuba, Berengut, Flambaum, Roberts (2012)

* Uncertainty was underestimated since important contributions were missed

Contributions missed in (*) were added.

Alkali atoms and similar ions (**Cs**, **Ba^+**, **Fr**, **Ra^+**, etc.) are the best for accurate calculations because of their simple electron structure (one electron above closed shells).

For accurate theoretical results one needs to include

- Many-body effects,
- Breit,
- QED.

Main challenge comes from many-body effects:

- ***Core polarization*** (change of core and its potential by external field). Can be treated within **RPA** (Hartree-Fock in external field).

- ***Correlations*** (beyond mean field wave function).
  Can be treated by correlation potential (CP) method with an all-order correlation potential Σ.

Two different approaches to calculations

- *Direct summation* approach (Johnson, Derevianko, Safronova)

$$E_{PV}(6s \to 7s) = \sum_n \left[\frac{\langle 7s | H_{PV} | nP \rangle \langle nP | D | 6s \rangle}{E_{7s} - E_{nP}} + \frac{\langle 7s | D | nP \rangle \langle nP | H_{PV} | 6s \rangle}{E_{6s} - E_{nP}} \right] = \xi Q_W$$

- *Solving equations* approach (used in our group):

$$E_{PNC} = \left\langle \delta\psi^{Br}_{6s} | D | \psi^{Br}_{7s} \right\rangle + \left\langle \psi^{Br}_{6s} | D | \delta\psi^{Br}_{7s} \right\rangle + \left\langle \psi^{Br}_{6s} | \delta V_{DW} | \psi^{Br}_{7s} \right\rangle$$

$\left(H_0 - E_v + \Sigma\right)\psi^{Br}_v = 0$ - Eq. for Brueckner orbitals

$\left(H_0 - E_v + \Sigma\right)\delta\psi^{Br}_v = -(F + \delta V_F)\psi^{Br}_v$ - **RPA** equations

F is weak or *D* or both

Σ is the correlation potential

Solving equations approach

PV amplitude in **RPA**

$$E_{PV}(6s-7s)=\langle\psi_{7s}\,|\,D+\delta V_D\,|\,\delta\psi_{6s}\rangle+\langle\psi_{7s}\,|\,W+\delta V_W\,|\,X_{6s}\rangle+\langle\psi_{7s}\,|\,\delta V_{DW}\,|\,\psi_{6s}\rangle$$

Double CP term
(-0.26% in Cs) missed
in many other calculations.

$\delta\psi, X, Y$ are corrections due to external field

Weak interaction (*W*): $\psi_a=\psi_{0a}+\delta\psi_a$

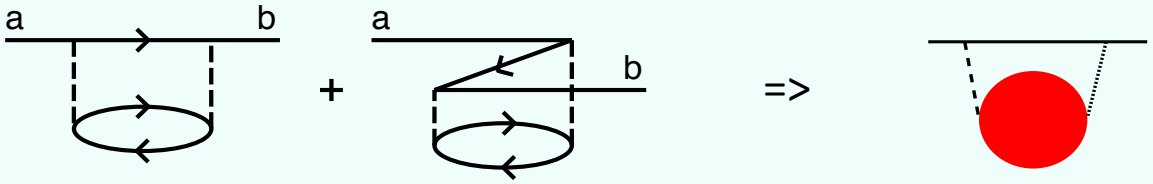
Electric field of external photon (*D*): $\psi_a=\psi_{0a}+X_a e^{-i\omega t}+Y_a e^{i\omega t}$

Both: $\psi_a=\psi_{0a}+\delta\psi_a+X_a e^{-i\omega t}+Y_a e^{i\omega t}+\delta X_a e^{-i\omega t}+\delta Y_a e^{i\omega t}$

$$\text{RPA:}\quad\left(H^{HF}-\varepsilon_a\right)\delta\psi_a=-\left(F+\delta V\right)\psi_{0a}$$

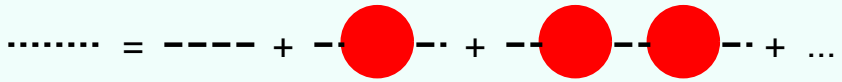
All-order correlation potential Σ.

2nd order Σ:

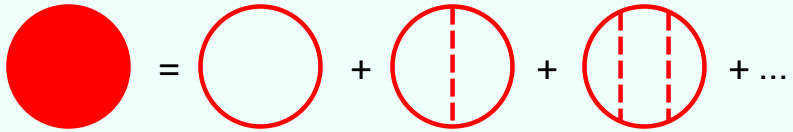


Four chains of higher-order diagrams are included:

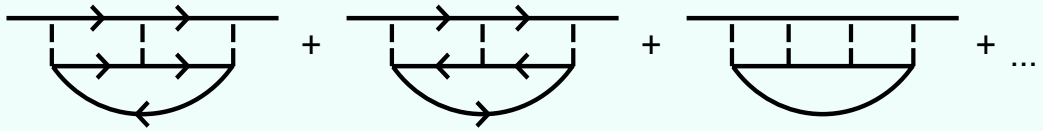
1. Screening of Coulomb interaction
(similar to screening of external electric field, i.e. Schiff theorem: *E(0)=0*).



2. Hole-particle interaction
(responsible for discrete spectrum of Noble gases).

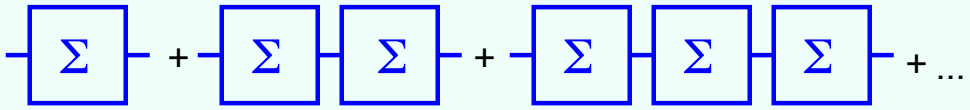


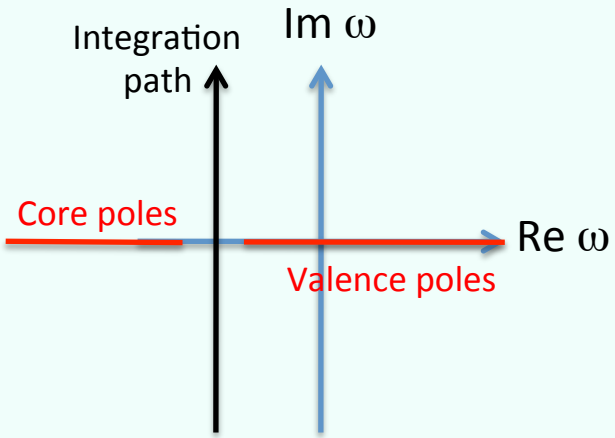
3. Ladder diagrams
(all-order residual Coulomb interaction of external electron with the core).



4. Iterations of **Σ**

$$(H^{HF} + \Sigma - \varepsilon)\psi = 0$$





$$\Sigma(r_1,r_2) = \int G_\omega(r_1,r_2)P_\omega(r_1,r_2)d\omega$$

G – Green function, *P* – polarization operator

$$(H_0 - \omega)G_\omega(r_1,r_2) = -\delta(r_1 - r_2)$$

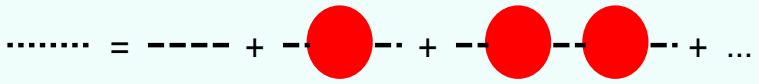
Without exchange:

$$G_0(r_1,r_2) = \psi_0(r_1)\psi_\infty(r_2)$$

With exchange:

$$G = G_0\left(1 - G_0 V_{ex}\right)^{-1}$$

Polarization operator:



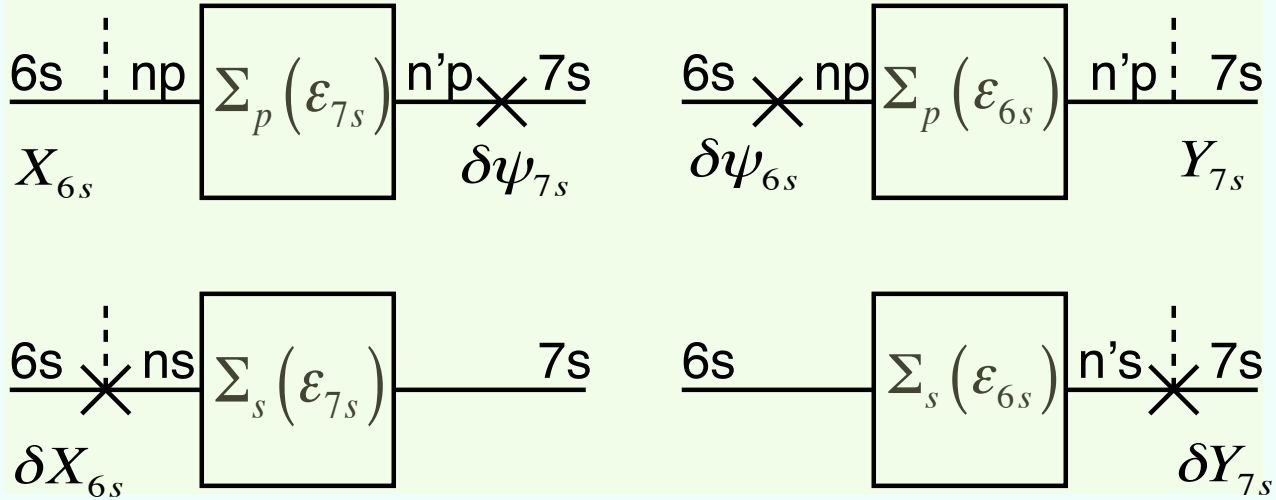
$$P = Q\Pi Q + Q\Pi Q\Pi Q + \ldots = Q\Pi Q(1 - \Pi Q)^{-1}$$

Matrix geometric progression!

P, Q, Π, G are matrixes in coordinate space

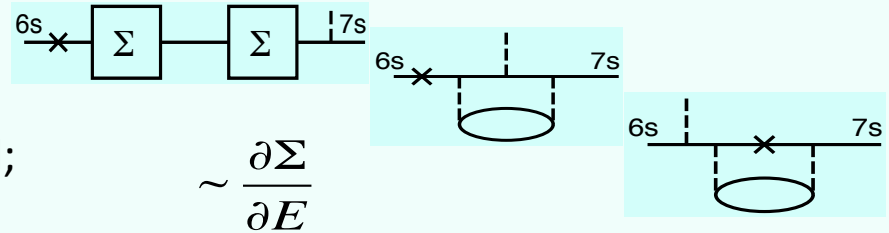
$$p_{ij} = P(r_i,r_j) \qquad \int \Pi(r_1,r)Q(r,r_2)dr \to \sum_k \pi_{ik}q_{kj}$$

Dominating correlation corrections to the PV amplitude



Other correlations corrections:

- Higher-order in **Σ** terms;
- Structure radiation;
- Weak correlation potential;
- Renormalization.



$$\sim \frac{\partial \Sigma}{\partial E}$$

Accuracy analysis

- *Solving equations* approach

$$E_{PNC} = \left\langle \delta\psi^{Br}_{6s} \,|\, D \,|\, \psi^{Br}_{7s} \right\rangle + \left\langle \psi^{Br}_{6s} \,|\, D \,|\, \delta\psi^{Br}_{7s} \right\rangle + \left\langle \psi^{Br}_{6s} \,|\, \delta V_{DW} \,|\, \psi^{Br}_{7s} \right\rangle$$

Need to check accuracy for two terms (third is small, ~-0.26% of E_{PNC})
Checking is done by using the same wavefunctions and Σ to calculate energies, E1 amplitudes, hfs, etc.
We have ~0.1% for EL and <0.5% for E1 and hfs.
We claim 0.5% for PNC.

- *Direct summation* approach

$$E_{PV}(6s \to 7s) = \sum_n \left[\frac{\langle 7s \,|\, H_{PV} \,|\, nP \rangle \langle nP \,|\, D \,|\, 6s \rangle}{E_{7s} - E_{nP}} + \frac{\langle 7s \,|\, D \,|\, nP \rangle \langle nP \,|\, H_{PV} \,|\, 6s \rangle}{E_{6s} - E_{nP}} \right] = \xi Q_W$$

Need to check accuracy for ~100 terms.
High accuracy for leading terms does not guarantee high accuracy for the sum.

$$E_{PV}(6s \to 7s) = \sum_n \left[\frac{\langle 7s | H_{PV} | nP \rangle \langle nP | D | 6s \rangle}{E_{7s} - E_{nP}} + \frac{\langle 7s | D | nP \rangle \langle nP | H_{PV} | 6s \rangle}{E_{6s} - E_{nP}} \right] = \zeta Q_W$$

nP states are divided into three groups:

1. Core (2p, 3p, 4p, 5p);
2. Main (6p, 7p, 8p, 9p give ~ 98% of the sum);
3. Tail (n>9).

Accuracy estimation for the core and tail terms:

Apply different approaches, use average as central point and scattering of the results as uncertainty estimate.
Problem: if something is missed in all approaches there is no way to see it!

Accuracy estimation for the main term:

Compare electric dipole amplitudes $\langle np|D|n's\rangle$ and energies with experiment;

Compare $\langle np|H_{PV}|n's\rangle$ with $\sqrt{A_p A_s}$ (hfs).

Accuracy of the hfs test for weak matrix elements is limited.

Sensitivity to many-body effects:

Approximation	Ratio hfs/weak	Change (%)
DHF	849	
RPA	822	-3
Brueckner (with Σ)	835	-1.5
Brueckner + RPA	810	-5

Accuracy of integration:

Number of points inside the nucleus	Change of weak matrix element (%)	Change of hfs
140	0	0
35	0.0034	0.0015
24	0.33	0.0066
18	2.1	0.010

Correlations for P-states

$$E_{PV}(6s \to 7s) = \sum_n \left[\frac{\langle 7s | H_{PV} | nP \rangle \langle nP | D | 6s \rangle}{E_{7s} - E_{nP}} + \frac{\langle 7s | D | nP \rangle \langle nP | H_{PV} | 6s \rangle}{E_{6s} - E_{nP}} \right] = \xi Q_W$$

$$\left(H_0 - E + \Sigma_p(\varepsilon) \right) \psi_p^{Br} = 0$$

To compare matrix elements with experiment we need $\Sigma_p\left(\varepsilon = \varepsilon_{np}\right)$

To calculate PNC we need $\Sigma_p\left(\varepsilon = \varepsilon_{6s}\right)$ and $\Sigma_p\left(\varepsilon = \varepsilon_{7s}\right)$

I.e, what is tested is not exactly what is needed.

$$E_{PNC} = \left\langle \delta\psi^{Br}_{6s} \,|\, D \,|\, \psi^{Br}_{7s} \right\rangle + \left\langle \psi^{Br}_{6s} \,|\, D \,|\, \delta\psi^{Br}_{7s} \right\rangle + \left\langle \psi^{Br}_{6s} \,|\, \delta V_{DW} \,|\, \psi^{Br}_{7s} \right\rangle$$

$$E_{PV}(6s \to 7s) = \sum_n \left[\frac{\langle 7s \,|\, H_{PV} \,|\, nP \rangle \langle nP \,|\, D \,|\, 6s \rangle}{E_{7s} - E_{nP}} + \frac{\langle 7s \,|\, D \,|\, nP \rangle \langle nP \,|\, H_{PV} \,|\, 6s \rangle}{E_{6s} - E_{nP}} \right] = \xi Q_W$$

To compare the calculations term by term we modify the wave functions:

$$\delta\psi \to \delta\psi - \left\langle \delta\psi \,|\, \psi_{np} \right\rangle \psi_{np}$$

(n=2,…,5 for the core,
n=6,…,9 for the main term,
what is left is the tail)

	A (Porsev et al) Sum over states	B (Dzuba et al) Solving equations	B - A
Core	-0.0020	0.0018	0.0038
Main	0.8823	0.8678	N/A
Tail	0.0195	0.0242	0.0047
Total	0.8998	0.8938	0.0085

- RPA is missed in A

-Not clear
(no details in A)

What about DCP? $\left\langle \psi^{Br}_{6s} \,|\, \delta V_{DW} \,|\, \psi^{Br}_{7s} \right\rangle$

Its contribution (0.0024) is equal to Uncertainty claimed in A.
But is it included?

The implication to neutron skin

Experimental accuracy for **Cs** is **0.35%**.
Theoretical accuracy for **Cs** is **0.44%**.

Similar theoretical accuracy can be achieved for **Rb**, **Ba^+**, **Fr**, **Ra^+**
(one electron above closed shells).

Atom	$K\Delta R_{np}/R_p$
^{133}Cs	-0.0026(5)
^{138}Ba	-0.0030(6)
^{221}Fr	-0.0070(16)
^{222}Ra	-0.0068(16)

Then **Fr** and **Ra^+** the are the best candidates to study neutron skin.
Fr: TRIUMF, Canada;
Ra^+: KVI, the Netherlands.

Other atoms considered for PV measurements (**I, Xe, Sm, Dy, Yb, Hg, Tl, Pb, Bi, Th**) have complicated electron structure resulting in insufficient theoretical accuracy (they can be used in the ***chain of isotopes*** measurements).

S-D PV transitions (e.g., the 6s-$5d_{3/2}$ transition in Ba^+).

The PV amplitude

$$E_{PV}(6s \to 5d) = \sum_n \left[\frac{\langle 5d | H_{PV} | np \rangle \langle np | D | 6s \rangle}{E_{5d} - E_{np}} + \frac{\langle 5d | D | np \rangle \langle np | H_{PV} | 6s \rangle}{E_{6s} - E_{np}} \right] = \xi Q_W$$

is strongly dominated by a single term

$$E_{PV}(6s \to 5d) \approx \frac{\langle 5d | D | 6p \rangle \langle 6p | H_{PV} | 6s \rangle}{E_{6s} - E_{6p}}$$

~ 80% of the sum.

If experimental data is used for $\langle 5d | D | 6p \rangle$ and theoretical for $\langle 6p | H_{PV} | 5d \rangle$,
High accuracy can be achieved.

The same is true for **Ra^+**!

The neutron skin contribution is -0.3% for **Ba^+** and -0.7% for **Ra^+**.

Isotopic ratios.

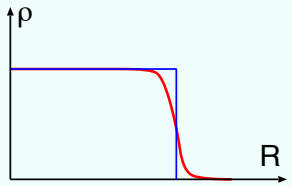
$$E_{PV} = K_{PV} Q_W$$

K_{PV} cancels out in the ratio $E_{PV}(A1)/E_{PV}(A2)$
(Dzuba, Flambaum, Khriplovich, Z. Phys. D **1**, 243 (1986)).

More accurately

$$\frac{E_{PV}(A_2)}{E_{PV}(A_1)} = \left(\frac{R_{2p}}{R_{1p}}\right)^{\beta} \frac{Q_{2W}}{Q_{1W}} \left[1 + K\left(\frac{\Delta R_{2np}}{R_{2p}} - \frac{\Delta R_{1np}}{R_{1p}}\right)\right]$$

[Neutron skin contribution]



$$\beta \approx 2\gamma - 2, \quad \gamma = \sqrt{1-(\alpha Z)^2}$$

The uncertainties due to R_p and Q_w are small, e.g.

$$\delta\left(\frac{R_{2p}}{R_{1p}}\right)^{\beta} \approx \beta \frac{(R_{p2} - R_{p1})\delta R_{p1}}{R_{1p}^2} < 10^{-4}$$

Change due to β instead of 2γ-2 ~ 2 x 10^{-4}.

	β	2γ-2
Cs	-0.182	-0.168
Ba	-0.188	-0.175
Dy	-0.266	-0.247
Yb	-0.302	-0.281
Fr	-0.489	-0.455
Ra	-0.502	-0.467

Taking ΔR_{np} from Brown et al, PRC **79**, 035501 (2009) leads to

Atom	Stable isotopes	Unstable (τ>1 day)	Neutrom skin correction
Cs	133	129-137	0.0012(2)
Ba	130-138	128-140	0.0012(2) -> 0.0018(2)
Sm	144-154	144-154	**0.0024(3)**
Dy	156-164	154-166	0.0012(3) -> 0.0018(3)
Yb	168-176	166-176	**0.0017(4)**
Hg	196-204	194-204	**0.0016(5)**
Tl	203,205	200-205	0.0004(5) -> 0.0010(5)
Pb	204-208	202-210	0.0008(5) -> 0.0016(5)
Bi	209	205-210	0.0010(5)
Fr		213-227 (τ>1m)	**0.0028(5)**
Ra		223-228	**0.0029(5)**

$$K\left(\frac{\Delta R_{2np}}{R_{2np}} - \frac{\Delta R_{1np}}{R_{1np}}\right)$$

Best candidates (in **bold**): **Sm, Yb, Hg, Fr, Ra**.

The ratio $A_{PV}(A_1)/A_{PV}(A_2)$ needs to be measured to **~10^{-3}** accuracy.

Neutron skin vs new physics

Atomic PV can be used in search for new physics if neutron skin is small or known from independent sources.

A. Single isotope measurements.

^{133}Cs: ΔR_{np} =0.13(4) fm from antiprotonic data,

Trzcinska *et al*, PRL **87**, 082501 (2001).

ΔR_{np} =0.158(37) fm from nuclear calculations,

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

Experiment:

$$-\mathrm{Im}(E_{PV})/\beta = 1.5935(1 \pm 0.35\%)\mathrm{mV/cm}$$

Wood *et al*, Science **275**, 1759 (1997).

Theoretical PV amplitude in Cs [$10^{-11}\, i(-Q_W/N)$ a.u.]

Contribution	**Value**
Many-body	0.9079(40)
Breit	-0.055(1)
QED	-0.0029(3)
Neutron skin	-0.0018(5)
Total	**0.8977(40)**

- Two times smaller than theoretical uncertainty

Comparing theoretical and experimental data tests SM and constrains new physics.

Using experimental values for E_{PV}/β and β
[β=26.957(51) a.u. Bennet and Wieman, PRL **82**, 2484 (1999)]

leads to $Q_W(^{133}Cs)=-72.58(29)_{exp}(32)_{theor}$,
while $Q_W^{SM}=-73.23(2)$.

$\Delta Q_W = Q_W - Q_W^{SM} = 0.65(43)$ 1.5σ

Using $\Delta Q_W = -0.800S - 0.007T$ [Rosner, PRD **65**, 073026 (2002)]
leads to $S=-0.81(54)$.

Using $\Delta Q_W = 0.4(2N+Z)(M_W/M_{Z\xi})^2$
[Marciano and Rosner, PRL **65**, 2963 (1990)]
leads to $M_{Z\xi}$ >710 GeV.

Another way of describing new physics

$\Delta Q_{new} = N h_n + Z h_p$

For cesium

$78 h_n + 55 h_p = 0.65(43)$.

This leads to $|h_n| < 0.014$; $|h_p| < 0.020$.

The single-isotope measurements are more sensitive to h_n.

Similar or better results can be obtained for Rb, Ba^+, Fr, Ra^+.

Atom	PV transition	Value [10^{-12} $iea_0(-Q_w/N)$]	Neutron skin	Where
^{85}Rb	[Kr]5s – [Kr]6s	1.39	0.07%	TRIUMF(?)
^{133}Cs	[Xe]6s – [Xe]7s	8.97	0.2%	Boulder, 1997
$^{138}Ba^+$	[Xe]6s – [Xe]$5d_{3/2}$	21.7	0.3%	Seattle
^{221}Fr	[Rn]7s – [Rn]8s	159	0.7%	TRIUMF
$^{222}Ra^+$	[Rn]7s – [Rn]$6d_{3/2}$	429	0.7%	KVI

Expected theoretical accuracy ~ 0.4% or better.

B. Isotope ratio measurements.

$$Q_W = Q_W^{SM} + \Delta Q_{\text{new}} \equiv h_0 N + h_p Z + h_n N$$

New physics

Single isotope measurements are sensitive to h_n.

Isotope ratio measurements are sensitive to h_p:

$$R = \frac{E_{1PV}}{E_{2PV}} = \frac{Q_{1W}}{Q_{2W}} \left(\frac{R_{1p}}{R_{2p}} \right)^{\beta} \approx R_0 \left(1 + \frac{Z \Delta N}{N_1 N_2} \frac{h_p}{h_0} \right)$$

R_0 is the ratio with no new physics.

Sensitivity function

$$F = \frac{h_p}{h_0} = \left(\frac{R}{R_0} - 1 \right) \frac{N_1 N_2}{Z \Delta N}$$

F=0 means no new physics.

Derevianko and Porsev, PRA 65, 052115 (2002).

The uncertainty δF comes from experiment (δR) and theory (δR_0),
The later is due to neutron skin:

$$F = \frac{h_p}{h_0} = \left(\frac{R}{R_0} - 1\right)\frac{N_1 N_2}{Z\Delta N} \qquad \delta F = \frac{h_p}{h_0} = \left(\frac{\delta R}{R_0} + K\frac{\delta \Delta R_n}{R_p}\right)\frac{N_1 N_2}{Z\Delta N}$$

Atom	A_1	A_2	δF_{NS} x10^3	h_p*
Cs	129	137	2.1	0.0020
Ba	130	138	2.3	0.0022
Sm	144	154	4.2	0.0039
Dy	156	164	2.7	0.0025
Yb	168	176	10.2	0.0096
Tl	203	205	7.2	0.0068
Pb	204	208	7.7	0.0072
Fr	209	221	8.8	0.0084
Ra	210	222	8.9	0.0084

Q^p_W=0.064(12);
Q_{weak} collaboration,
PRL **111**, 141803 (2013);

=> h_p<0.012.

Isotope chain measurements are competitive to the PVES measurements!

Cs, Ba and **Dy** are the best candidates.

* Limits on h_p from nuclear skin uncertainty.

Summary

Atomic PV measurements can be used to study neutron skin and to search for new physics.

Single isotope measurements		
	Neutron skin	**New physics**
Sensitive to	ΔR_{np}	h_n
Theoretical accuracy	<1%	<1%
Experimental accuracy	<1%	<1%
Best candidates	Fr, Ra^+	Rb, Cs, Ba^+, Fr, Ra^+
Isotope ratio measurements		
Sensitive to	$\delta\Delta R_{np}$	h_p
Theoretical accuracy	N/A	N/A
Experimental accuracy	~10^{-3}	~10^{-3}
Best candidates	Fr, Ra^+, Yb	Rb, Cs, Ba^+, Dy