Time and parity invariance violations in heavy atoms

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Overview

- Atoms as probes of fundamental interactions
  - *atomic electric dipole moments (EDMs)*
  - Nuclear Schiff moment
  - *atomic parity violation (APV)*

    - nuclear weak charge

    - nuclear anapole moment
- High-precision atomic many-body calculations
- EDMs of diamagnetic atoms
- Strong enhancement of SM in deformed nuclei
- Strong enhancement of EDMs and APV due to close levels of opposite parity: Ra, Rare Earth
- APV in Cs, QED corrections
- Summary

Atoms as probes of fundamental interactions

- T,P and P-odd effects in atoms are strongly enhanced:
  - Z^3 or Z^2 electron structure enhancement (universal)
  - Nuclear enhancement (mostly for non-spherical nuclei)
    - Close levels of opposite parity
    - Collective enhancement
    - Octupole deformation
  - Close atomic levels of opposite parity (mostly for excited states)

- A wide variety of effects can be studied:

Schiff moment, MQM, nucleon EDM, e^- EDM via atomic EDM
Q_W, Anapole moment via *E(PNC)* amplitude

Atomic EDMs

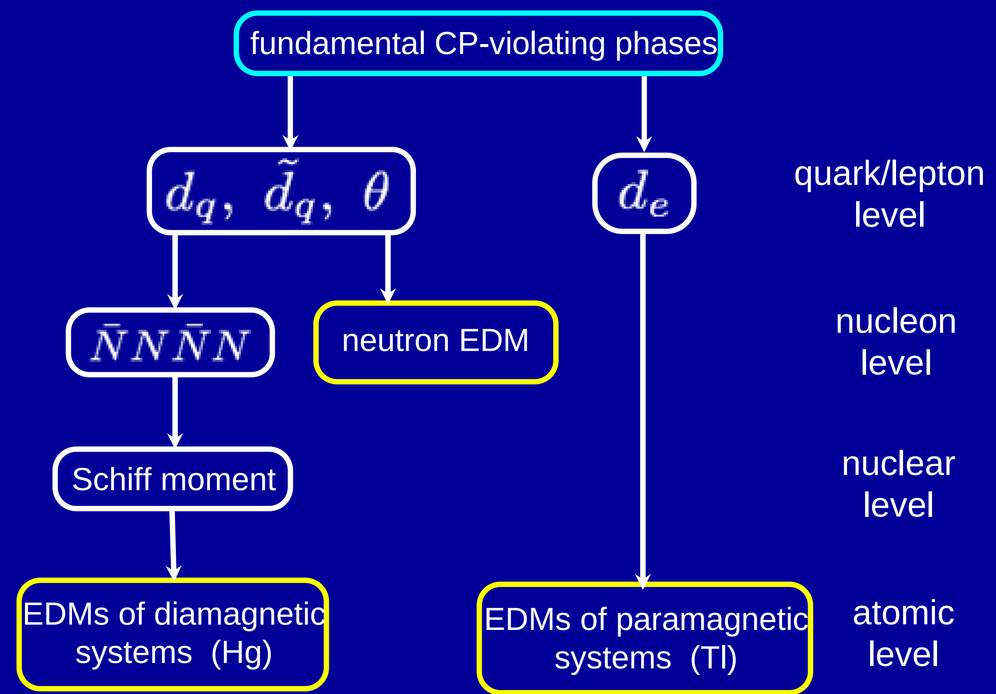
Best limits

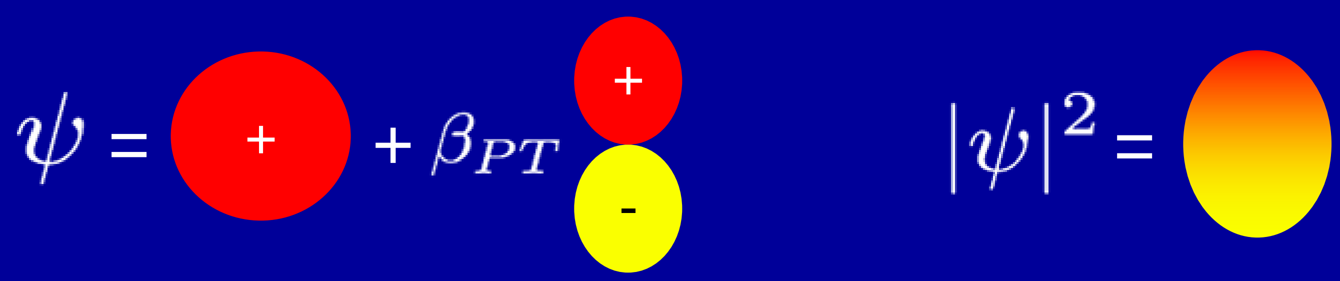
$|d(^{199}\text{Hg})| < 2.1 \times 10^{-28}\ e$ cm
(95% c.l., Seattle, 2001)

$|d(^{205}\text{Tl})| < 9.6 \times 10^{-25}\ e$ cm
(90% c.l., Berkeley, 2002)

$|d(\text{n})| < 2.9 \times 10^{-26}\ e$ cm
(90% c.l., Grenoble, 2006)

Leading mechanisms for EDM generation





- Excellent way to search for new sources of CP-violation is by measuring EDMs
  - SM EDMs are hugely suppressed
  - → Theories that go beyond the SM predict EDMs that are many orders of magnitude larger!

e.g. electron EDM [Commins]

Theory	d_e (e cm)
Std. Mdl.	$< 10^{-38}$
SUSY	10^{-28} - 10^{-26}
Multi-Higgs	10^{-28} - 10^{-26}
Left-right	10^{-28} - 10^{-26}

Best limit (90% c.l.): $|d_e| < 1.6 \times 10^{-27}$ $e\ cm$ Berkeley (2002)

- Atomic EDMs $d_{atom} \propto Z^2, Z^3$ [Sandars]

Sensitive probe of physics beyond the Standard Model!

Schiff moment

SM appears when screening of external electric field by atomic electrons is taken into account.

Nuclear T,P-odd moments:

- EDM – non-observable due to total screening
- Electric octupole moment – modified by screening
- Magnetic quatrupole moment – not significantly affected

Nuclear electrostatic potential with screening:

$$\varphi(\mathbf{R}) = \int \frac{e\rho(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|} d^3r + \frac{1}{Z}(\mathbf{d} \bullet \nabla) \int \frac{\rho(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|} d^3r$$

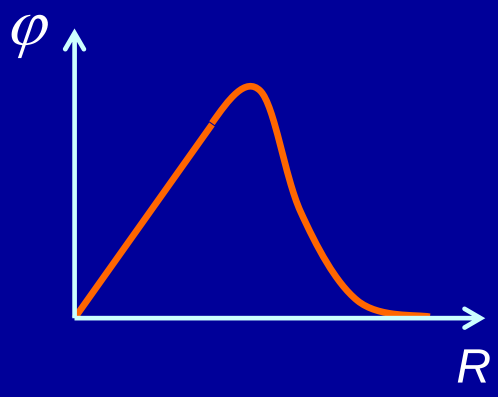
d is nuclear EDM, the term with **d** is the electron screening term

φ(**R**) in multipole expansion is reduced to $\varphi(\mathbf{R}) = 4\pi \mathbf{S} \bullet \nabla \delta(\mathbf{R})$

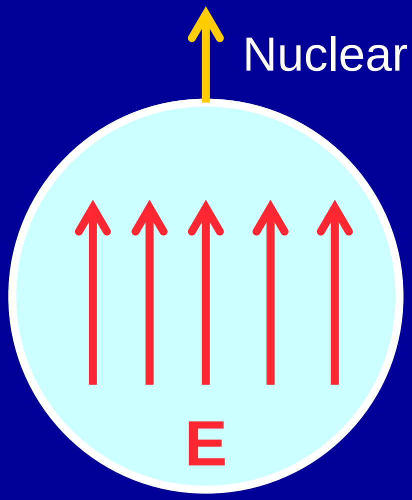
where $\mathbf{S} = \frac{e}{10}\left[\left\langle r^2\mathbf{r}\right\rangle - \frac{5}{3Z}\left\langle r^2\right\rangle\left\langle \mathbf{r}\right\rangle\right]$ is Schiff moment.

This expression is not suitable for relativistic calculations.

Flambaum, Ginges, 2002: $\varphi(\mathbf{R}) = -\frac{3\mathbf{S}\bullet\mathbf{R}}{B}\rho(R)$ where $B = \int \rho(R) R^4 dR$



Electric field induced by T,P-odd nuclear forces which influence proton charge density:



This potential has no singularities and may be used in relativistic calculations

SM electric field polarizes an atom and produces the EDM

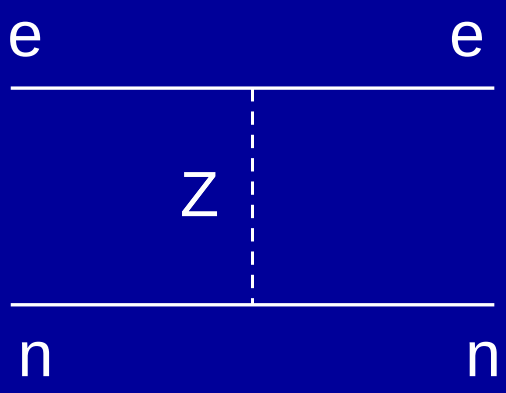
Relativistic corrections originating from electron wave functions can be incorporated into *Local Dipole Moment* (**L**)

$$\mathbf{L} = \sum_{k=1}^{\infty} \mathbf{S}_k$$

$$\varphi(\mathbf{R}) = 4\pi \mathbf{L} \bullet \nabla \delta(\mathbf{R})$$

Atomic parity violation

- Dominated by Z-boson exchange between electrons and nucleons



$$H = \frac{G}{\sqrt{2}}\left[C_{1p}\bar{e}\gamma_\mu\gamma_5 e\bar{p}\gamma^\mu p + C_{1n}\bar{e}\gamma_\mu\gamma_5 e\bar{n}\gamma^\mu n\right]$$

Standard model tree-level couplings: $C_{1p} = \frac{1}{2}\left(1 - 4\sin^2\theta_W\right) \;\; ; \;\; C_{1n} = -\frac{1}{2}$

- In atom with Z electrons and N neutrons obtain effective Hamiltonian parameterized by "nuclear weak charge" Q_W

$$h_{PV} = \frac{G}{2\sqrt{2}} Q_W \rho(r)\gamma_5$$

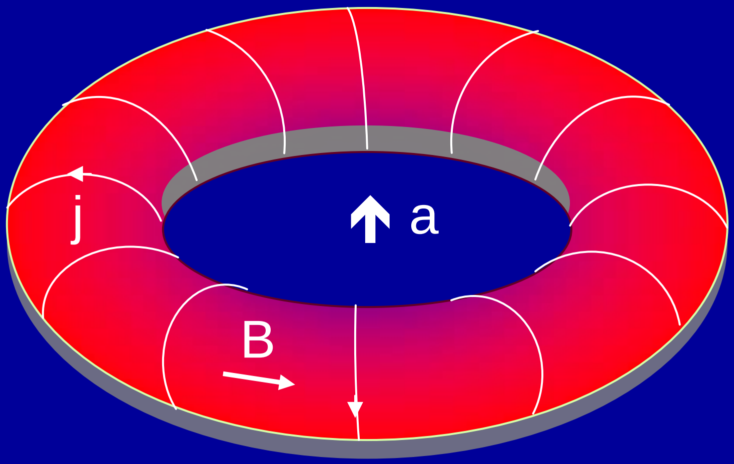
$$Q_W = 2(NC_{1n} + ZC_{1p}) \approx -N + Z(1 - 4\sin^2\theta_W) \approx -N$$

- APV amplitude $E_{PV} \propto Z^3$ [Bouchiat,Bouchiat]

Clean test of standard model via atomic experiments!

Nuclear anapole moment

- Source of nuclear spin-dependent PV effects in atoms
- Nuclear magnetic multipole violating parity
- Arises due to parity violation inside the nucleus



- Interacts with atomic electrons via usual magnetic interaction (PV hyperfine interaction):

$$h_a = e\vec{\alpha}\cdot\vec{A} \propto \kappa_a \vec{\alpha}\cdot\vec{I}\rho(r)\,, \quad \kappa_a \propto A^{2/3}$$

[Flambaum,Khriplovich,Sushkov]

$E_{PV} \propto Z^2 A^{2/3}$ measured as difference of PV effects for transitions between hyperfine components

- Boulder Cs: **g= 6(1)** (in units of Fermi constant)
- Seattle Tl: **g=-2(3)**

Atomic calculations

- APV

$$E_{PV}(1\rightarrow 2)=\sum_n\left[\frac{\langle 2|H_{PV}|n\rangle\langle n|D|1\rangle}{E_2-E_n}+\frac{\langle 2|D|nP\rangle\langle n|H_{PV}|1\rangle}{E_1-E_n}\right]=\zeta Q_W$$

- Atomic EDM

$$d_{atom}(1)=2\sum_n\frac{\langle 1|D_z|N\rangle\langle N|H_{PT}|1\rangle}{E_1-E_N}=\xi S$$

H_{PV} is due to electron-nucleon P-odd interactions,
H_{PT} is due to nucleon-nucleon, electron-nucleon PT-odd interactions, electron, proton or neutron EDM.

Atomic wave functions need to be good at *all* distances!

We check the quality of our wave functions by calculating:

- hyperfine structure constants and isotope shift
- energies
- E1 transition amplitudes

and comparing to measured values… there are also other checks!

Ab initio methods of atomic calculations

N_{ve}	Method	Accuracy
0	RHF+RPA	~ 10%
1	Correlation potential (Σ)	0.1-1%
2-8	CI+MBPT	1-10%
2-15	Configuration interaction	10-20%

N_{ve} *- number of valence electrons*

These methods cover all periodic table of elements

Correlation potential method

[Dzuba,Flambaum,Sushkov (1989)]

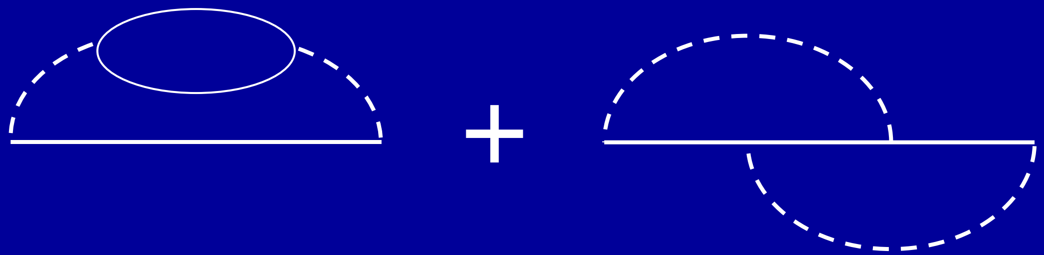
- Zeroth-order: relativistic Hartree-Fock. Perturbation theory in difference between exact and Hartree-Fock Hamiltonians.

- Correlation corrections accounted for by inclusion of a “correlation potential” Σ:

$$V_{HF} \rightarrow V_{HF} + \Sigma$$

In the lowest order Σ is given by:

$\Sigma =$

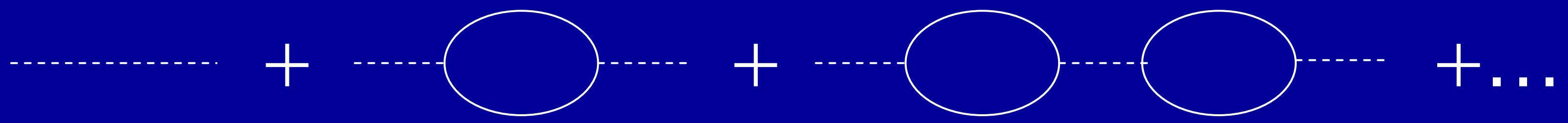


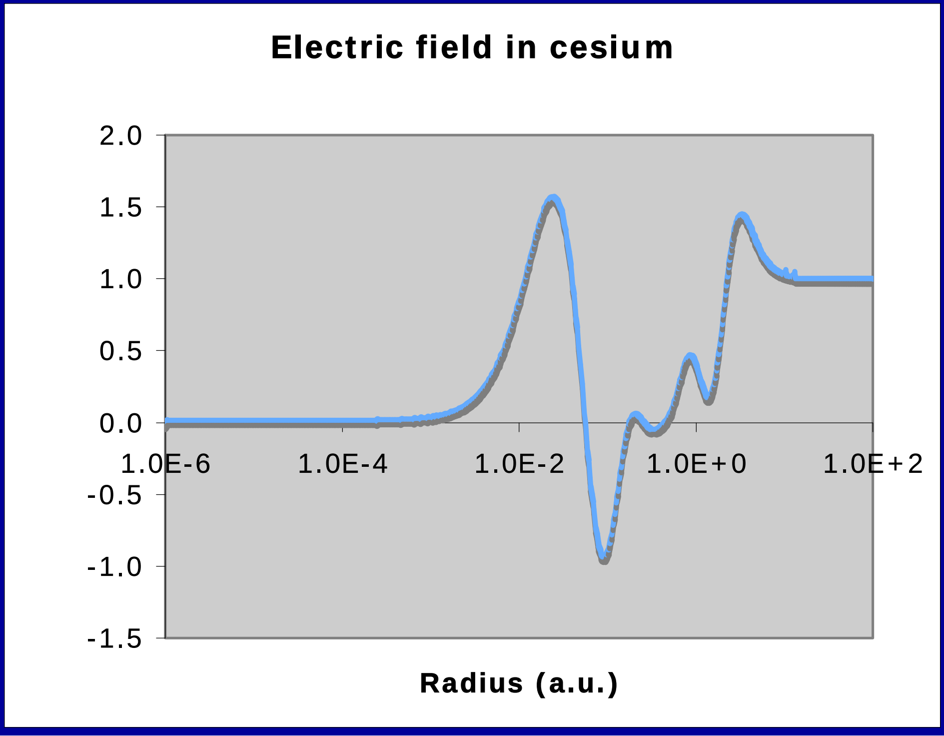
- External fields included using Time-Dependent Hartree-Fock (RPAE core polarization)+correlations

The correlation potential

Use the Feynman diagram technique to include three classes of diagrams to all orders:

1. electron-electron screening





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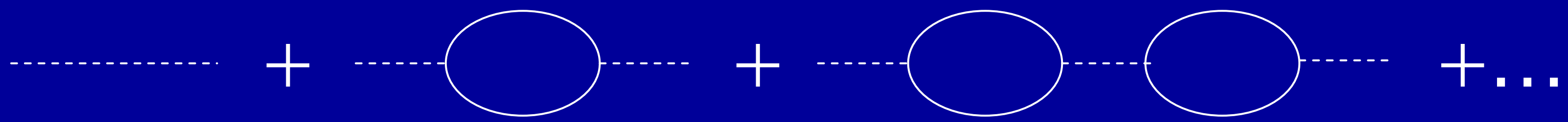
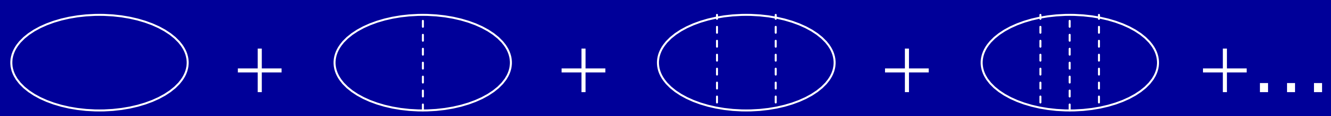
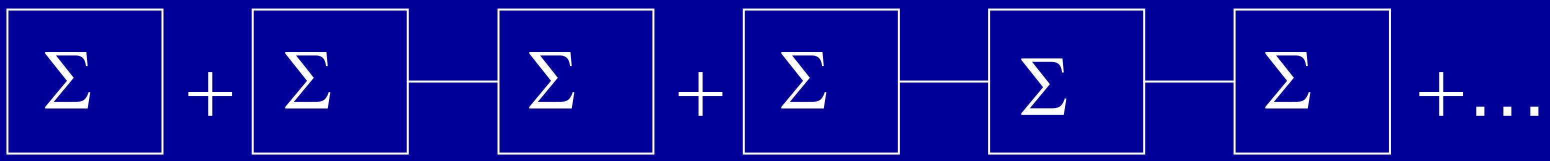


2. hole-particle interaction



3. nonlinear-in-Σ corrections



Matrix elements: $<\psi_a|h+\delta V+\delta\Sigma|\psi_b>$

$\psi_{a,b}$ - Brueckner orbitals: $(H^{HF}-\varepsilon_a+\Sigma)\psi_a=0$

h – External field

$<\psi_a|\delta V|\psi_b>$ - Core polarization

$<\psi_a|\delta\Sigma|\psi_b>$ - Structure radiation

Example: PNC *E(6s-7s)* in ^{133}Cs [$10^{-11} iea_B(-Q_W/N)$]

E_{PNC} = 0.91(1) (Dzuba, Sushkov, Flambaum, 1989)

E_{PNC} = 0.904(5) (Dzuba, Flambaum, Ginges, 2002)

Atoms with several valence electrons: CI+MBPT

[Dzuba, Flambaum, Kozlov (1996)]

CI Hamiltonian: $\Sigma_i h_i + \Sigma_{i<j} e^2/r_{ij}$

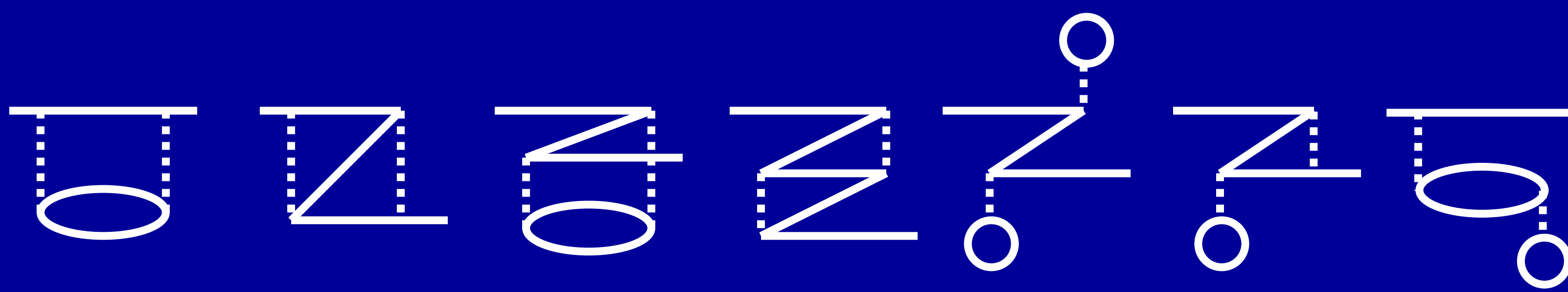
$h = c\boldsymbol{\alpha}\boldsymbol{p} + (\beta\text{-}1)mc^2 - Ze^2/r + V_{core}$

CI+MBPT Hamiltonian:

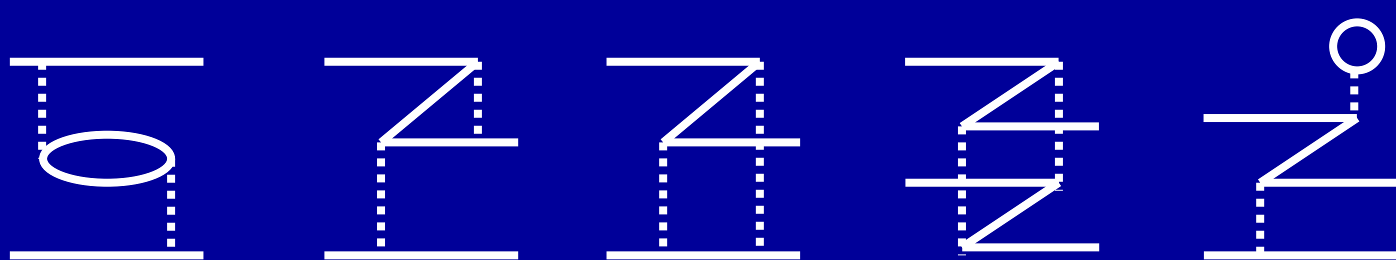
$h \text{ -> } h + \Sigma_1; \quad e^2/r_{ij} \text{ -> } e^2/r_{ij} + \Sigma_2$

MBPT is used to calculate core-valence correlation operator $\Sigma(r,r',E)$

Σ_1:



Σ_2:



Then standard CI technique is used:

Wave functions $$\Psi_a = \sum_i x_i^{(a)} \Phi_i$$

are found by solving matrix eigenvalue problem $$(H^{eff} - E)X = 0$$

Matrix elements are found by

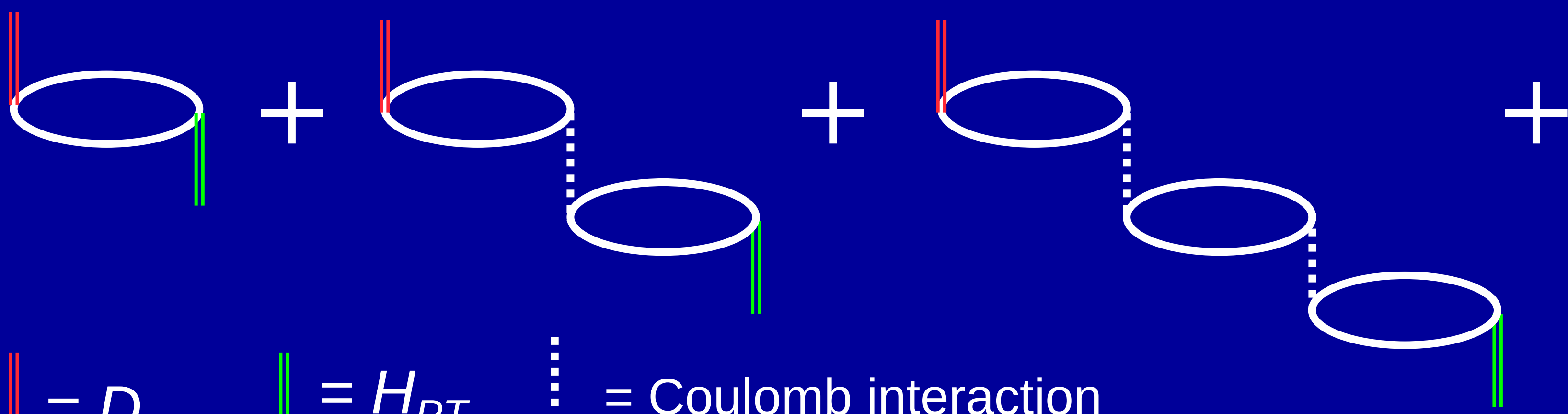
$$M_{ab} = \sum_{ij} x_i^{(a)} x_j^{(b)} \left\langle \Phi_i \,|\, \sum_{n=1}^{N_{VE}} (h + \delta V_{core} + \delta\Sigma)_{(n)} \,|\, \Phi_j \right\rangle$$

Example: EDM of Hg

EDM for closed-shell atoms
(Xe, Hg, Ra, Yb)
(due to Schiff moment)

$$d_{atom}(1) = 2\sum_N \frac{\langle 1|D_z|N\rangle\langle N|H_{PT}|1\rangle}{E_1 - E_N}$$

RHF + TDHF (for core polarization):



|| $= D_z$ || $= H_{PT}$ ⋮ = Coulomb interaction

Hg, Ra, Yb can also be treated as 2-valence electrons atoms by the CI+MBPT
The results for EDM are close to the RHF + TDHF calculations

EDMs of atoms of experimental interest

Z	Atom	[*S*/(e fm3)]*e* cm	[10^{-25} η] *e* cm	Expt.
2	^3He	0.00008	0.0005	
54	^{129}Xe	0.38	0.7	Seattle, Ann Arbor, Princeton
70	^{171}Yb	-1.9	3	Bangalore,Kyoto
80	^{199}Hg	-2.8	4	Seattle
86	^{223}Rn	3.3	3300	TRIUMF
88	^{225}Ra	-8.2	2500	Argonne,KVI
88	^{223}Ra	-8.2	3400	

$d_n = 5 \times 10^{-24}\, e$ cm η, $d(^3\text{He})/ d_n = 10^{-5}$

Limits on the P,T-violating parameters in the hadronic sector extracted from Hg compared to the best limits from other experiments

Best limit on atomic EDM (Seattle, 20001):

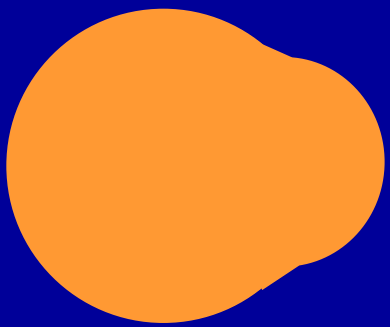
$d(^{199}Hg) = -(1.06 \pm 0.49 \pm 0.40) \times 10^{-28}\ e \cdot cm$

P,T-odd term	Value	Experiment	
neutron EDM d_n [10^{-26} *e* cm]	$(17 \pm 8 \pm 6)$ $(0.2 \pm 1.5 \pm 0.7)$ (1.9 ± 5.4) $(2.6 \pm 4.0 \pm 1.6)$	Hg n n n	Seattle, 2001 ILL, 2006 ILL, 1999 PNPI, 1996
proton EDM d_p [10^{-24} *e* cm]	$(1.7 \pm 0.8 \pm 0.6)$ (17 ± 28)	Hg TlF	Seattle, 2001 Yale, 1991
$\eta_{np} i \frac{G}{\sqrt{2}} \bar{p} p \bar{n} \gamma_5 n$	$\eta_{np} = (2.7 \pm 1.3 \pm 1.0) \times 10^{-4}$	Hg	Seattle, 2001
QCD phase θ [10^{-10}]	$(1.1 \pm 0.5 \pm 0.4)$ (1.6 ± 4.5) $(2.2 \pm 3.3 \pm 1.3)$	Hg n n	Seattle, 2001 ILL, 1999 PNPI, 1996

Nuclear enhancement

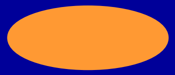
(Auerbach, Flambaum, Spevak (1996))

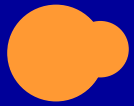
The strongest enhancement is due to octupole deformation (Ba-Sm; Ra-Th)



Intrinsic Schiff moment:

$$S_{\text{intr}} \approx eZR_N^3 \frac{9\beta_2\beta_3}{20\pi\sqrt{35}}$$

$\beta_2 \approx 0.2$ - quadrupole deformation 

$\beta_3 \approx 0.1$ - octupole deformation 

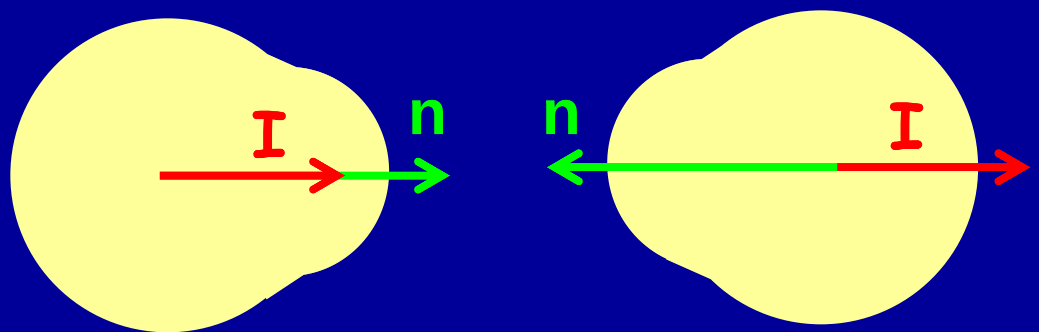
No T,P-odd forces are needed for the Schiff moment in intrinsic reference frame

However, in laboratory frame S=0 due to rotation

In the absence of T,P-odd forces

$$\Psi = \frac{1}{\sqrt{2}}\left(\left|IMK\right\rangle + \left|IM-K\right\rangle\right)$$

and $\langle \mathbf{n} \rangle = 0$



$$\mathbf{K} = (\mathbf{I} \bullet \mathbf{n})$$

With T,P-odd mixing (β):

$$\Psi = \frac{1}{\sqrt{2}}\left[(1+\beta)\left|IMK\right\rangle + (1-\beta)\left|IM-K\right\rangle\right]$$

and $\langle \mathbf{n} \rangle \propto \beta \mathbf{I}$

Schiff moment $\langle \mathbf{S} \rangle \propto \langle \mathbf{n} \rangle \propto \beta \mathbf{I}$

Simple estimate:

$$S_{lab} \propto \frac{\langle + | H_{TP} | - \rangle}{E_+ - E_-} S_{body}$$

Two factors of enhancement:

1. Large collective moment in the body frame
2. Small energy interval (E_+-E_-)

$$S \approx 0.05 e \beta_2 \beta_3^2 Z A^{2/3} \eta r_0^3 \frac{\mathrm{eV}}{E_+ - E_-} \approx 700 \times 10^{-8} \eta e \mathrm{fm}^3 \approx 500 S(\mathrm{Hg})$$

Engel, Friar, Hayes (2000); Flambaum, Zelevinsky (2003):
Static octupole deformation is not essential, nuclei with soft octupole vibrations also have the enhancement.

Extra enhancement in excited states: Ra

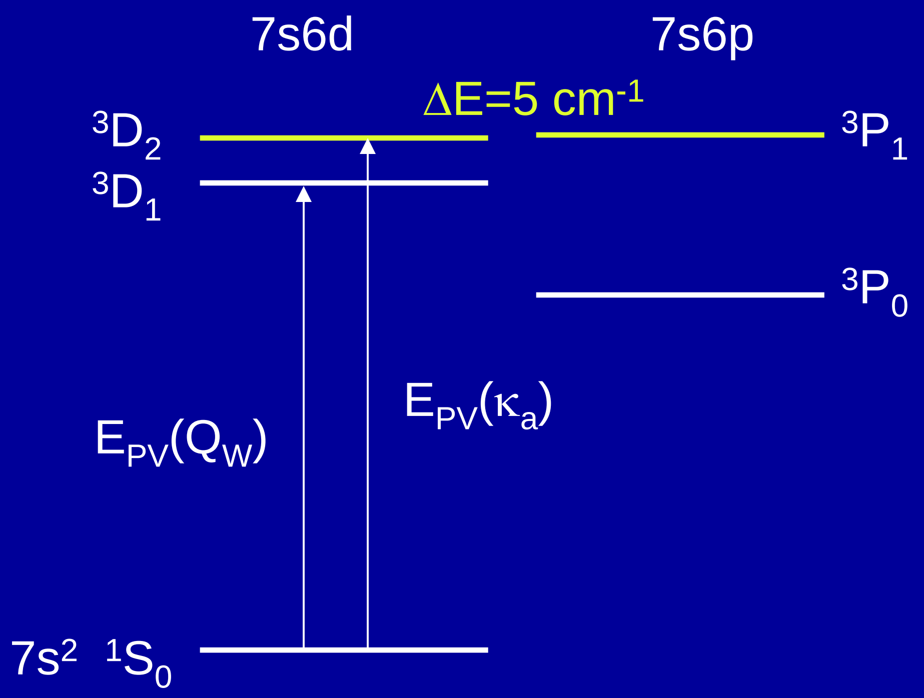
$$d_{atom}(1) = 2\sum_N \frac{\langle 1|D_z|N\rangle\langle N|H_{PT}|1\rangle}{E_1 - E_N}$$

- Extra enhancement for EDM and APV in metastable states due to presence of close opposite parity levels

  [Flambaum; Dzuba,Flambaum,Ginges]

$d(^3D_2) \sim 10^5 \times d(\mathrm{Hg})$

$E_{PV}(^1S_0\text{-}^3D_{1,2}) \sim 100 \times E_{PV}(\mathrm{Cs})$



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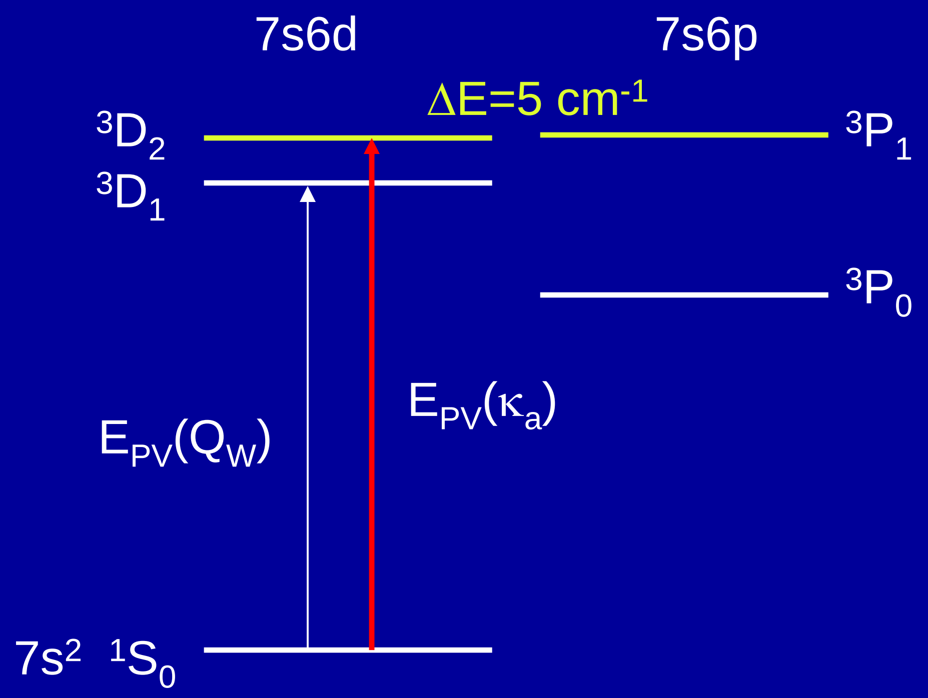


Good to study anapole moment:
- Strongly enhanced ($E_{PV} \sim 10^3\, E_{PV}$ (Cs))
- Q_W does not contribute ($\Delta J = 2$)

Close states of opposite parity in Rare-Earth atoms

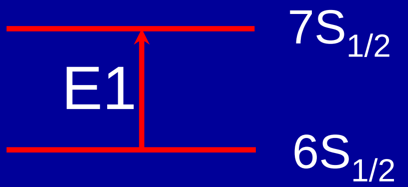
Z	Atom	Even	Odd	ΔE [cm^{-1}]	ΔJ	What
60	Nd II	$^6G_{11/2}$	$^6L_{13/2}$	8	1	S,M
62	SM I	$4f^6 5d6s$	$4f^6 6s6p$	5	0	S,E,M
62	SM I	$^7D_4$	$^9G_5$	10	1	S,M
64	Gd I	$^{11}F_5$	$^9P_3$	0	2	A,M
66	Dy I	$4f^{10} 5d6s$	$4f^{10} 6s6p$	1	1	A,S,M
66	Dy I	$4f^{10} 5d6s$	$4f^9 5d^2 6s$	0	0	A,E,S,M
67	Ho I	$^8K_{21/2}$	$4f^{10} 6s^2 6p$	10	1	S,M

S = Schiff Moment, A = Anapole moment, E = Electron EDM,
M = Magnetic quadrupole moment

PNC in Cs

- Best measurement for cesium [Boulder '97]

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



- Atomic theory required for determination of Q_W

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

Atomic theory	$\delta E_{PV}/E_{PV}$	$Q_W - Q_W^{SM}$	Ref.
1% calculations		1.2σ	Dzuba et al. '89; Blundell et al. '90
Reinterpretation 1% to 0.4%		2.5σ	Bennett & Wieman '99
Breit interaction	-0.6%		Derevianko '00
Vacuum polarization	+0.4%		Johnson et al. '01; Milstein & Sushkov '02
Neutron distribution	-0.2%		Derevianko '02
0.5% calculations		2.1σ	Dzuba, Flambaum, Ginges '02 Kozlov, Porsev, Tupitsyn, '01
Self-energy and vertex radiative corrections	-0.7%		Kuchiev & Flambaum '02; Milstein et al. '02; Sapirstein et al. '03; Shabaev et al. '05; Flambaum & Ginges '05
Total		1.1σ	

QED corrections to E_{PV} in Cs

$$E_{PV} = \sum_p \frac{W_{sp} E1_{ps}}{E_s - E_p}$$

QED correction to weak matrix elements leading to δE_{PV} (Kuchiev, Flambaum, '02; Milstein, Sushkov, Terekhov, '02; Sapirstein, Pachucki, Veitia, Cheng, '03)

δE_{PV} = (0.4-0.8)% = -0.4%

brings Cs PNC to agreement with the standard model

However, this not the end of the story

A complete calculation of QED corrections to PV *amplitude* includes also

- QED corrections to energy levels and E1 amplitudes and
- Many-body effects

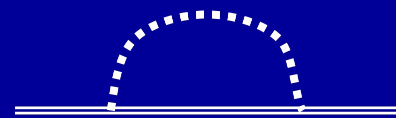
[Flambaum,Ginges; Shabaev,Pachuki,Tupitsyn,Yerokhin]

[Flambaum,Ginges, Dzuba]

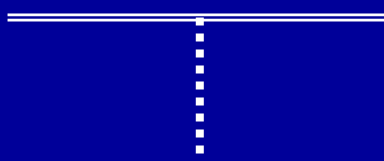
Radiative potential for QED

$$\Phi_{\rm rad}(r)=\Phi_U(r)+\Phi_g(r)+\Phi_f(r)+\Phi_l(r)+\frac{2}{3}\Phi_{WC}^{simple}(r)$$

$$\Phi_g(r)+\Phi_f(r)+\Phi_l(r)=$$



$$\Phi_U(r)+\frac{2}{3}\Phi_{WC}^{simple}(r)=$$



$\Phi_g(r)$ – magnetic formfactor
$\Phi_f(r)$ – electric formfactor (high frequency)
$\Phi_l(r)$ – electric formfactor (low frequency)
$\Phi_U(r)$ – Uehling potential
$\Phi_{WC}(r)$ – Wichmann-Kroll potential

$\Phi_f(r)$ and $\Phi_l(r)$ have free parameters which are chosen to fit QED corrections to the energies (Mohr, et al) and weak matrix elements (Kuchiev,Flambaum; Milstein,Sushkov,Terekhov; Sapirstein et al)

QED corrections to E_{PV} in Cs

$$E_{PV} = \sum_p \frac{W_{sp} E1_{ps}}{E_s - E_p}$$

- QED correction to weak matrix elements leading to δE_{PV} (Kuchiev, Flambaum, '02; Milstein, Sushkov, Terekhov, '02; Sapirstein, Pachucki, Veitia, Cheng, '03)

  δE_{PV} = (0.4-0.8)% = -0.4%

- QED correction to δE_{PV} in effective atomic potential (Shabaev *et al*, '05)

  δE_{PV} = (0.41-0.67)% = -0.27%

- QED corrections to *E1* and ΔE in radiative potential with full account of many-body effects, QED corrections to weak matrix elements are taken from earlier works (Flambaum, Ginges, '05)

  δE_{PV} = (0.41-0.73)%=-0.32%

- QED correction to δE_{PV} in radiative potential with full account of many-body effects (Dzuba, Flambaum, Ginges, '07)

  δE_{PV} = -0.21%

Cs PNC: conclusion and future directions

- Cs PNC is in good agreement with the standard model
- Tightly constrains possible new physics, e.g. mass of extra Z boson $M_{Z'} > 750$ GeV
- Theoretical uncertainty is now dominated by correlations (0.5%)
- Improvement in precision for correlation calculations is important. Derevianko aiming for 0.1% in Cs.
- Similar measurements and calculations can be done for Fr, Ba+, Ra+

Summary

- Precision atomic physics can be used to probe fundamental interactions
  - EDMs (existing): Xe, Tl, Hg
  - EDMs (new): Xe, Ra, Yb, Rn
  - EDM and APV in metastable states: Ra, Rare Earth
  - Nuclear anapole: Cs, Tl, Fr, Ra, Rare Earth
  - APV (Q_W): Cs, Fr, Ba+, Ra+
- Atomic theory provides reliable interpretation of the measurements