

September 20, 2007

Rare Isotopes & Fundamental symmetries workshop

ATOMIC PNC THEORY:
CURRENT STATUS AND
FUTURE PROSPECTS

MARIANNA SAFRONOVA



OUTLINE

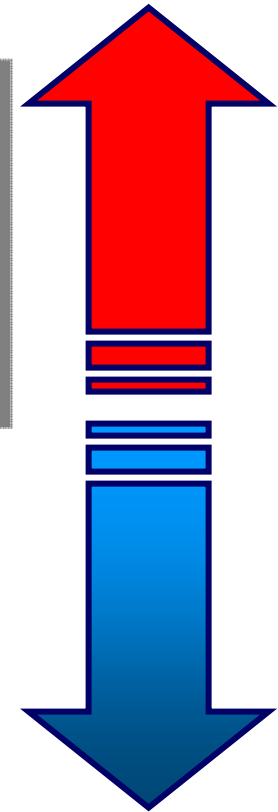
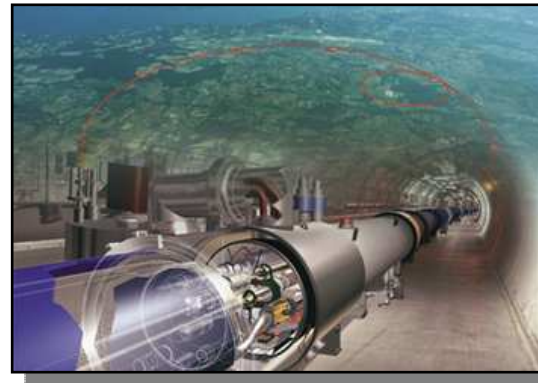
- Motivation & Summary of experiment
- Nuclear spin-independent PNC & weak charge
- How to determine the theoretical uncertainty?
- Nuclear spin-dependent PNC & anapole moments
- Overview of theoretical methods
- All-order method
- CI + all-order method & future prospects

MOTIVATION: PNC I

Searches for new physics beyond the Standard Model

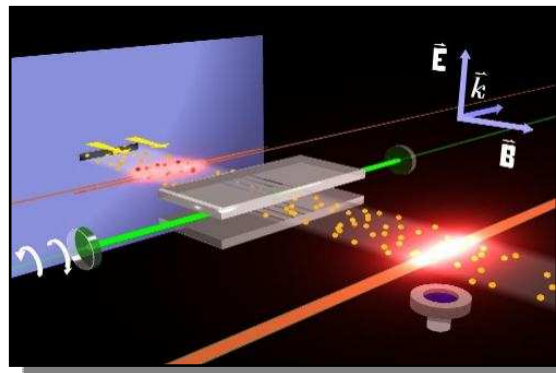
- (1) Search for new processes or particles directly
- (2) Study (**very precisely!**) quantities which Standard Model predicts and compare the result with its prediction

High energies



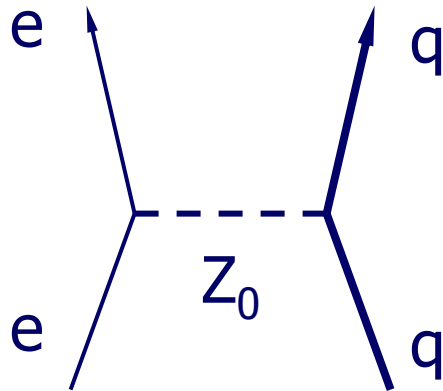
Low energies

Weak charge Q_W



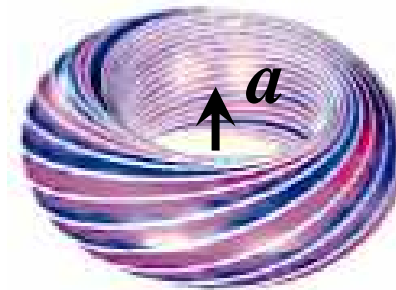
MOTIVATION: PNC

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



Weak Charge Q_W

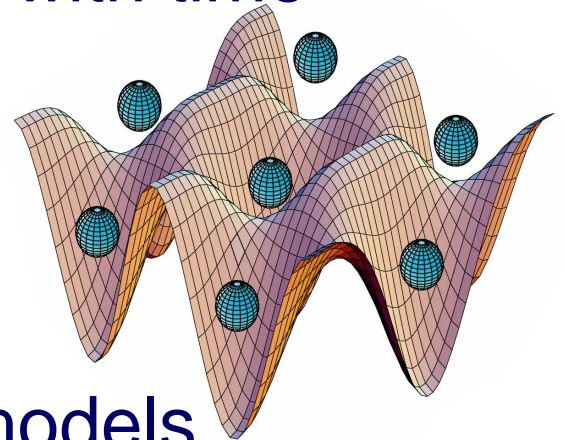
NUCLEAR
SPIN-DEPENDENT
PNC:
STUDY OF PNC
IN THE NUCLEUS



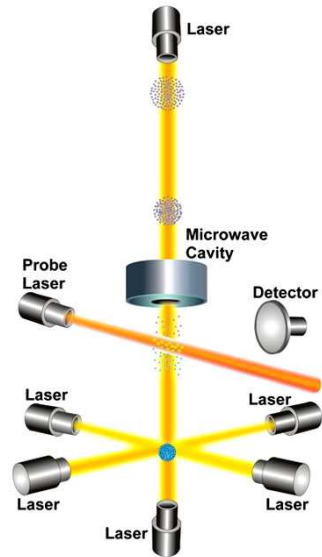
Nuclear anapole
moment

MOTIVATION: OTHER

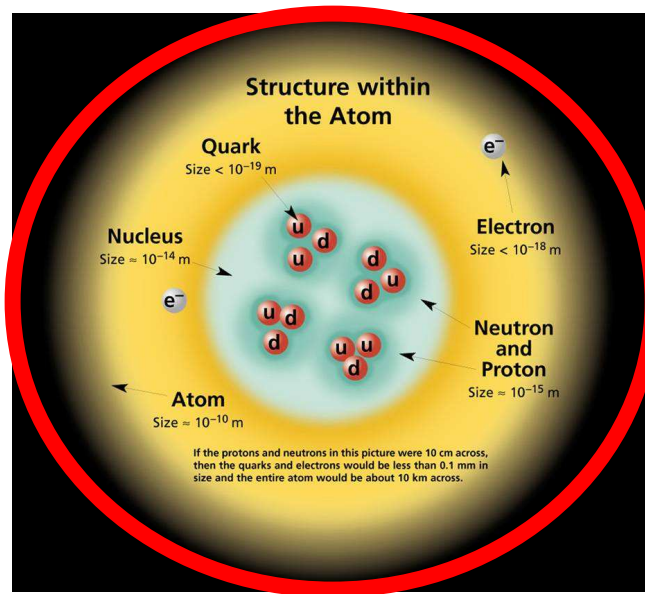
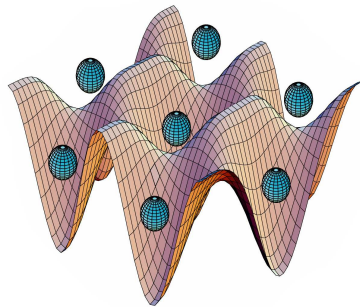
- Benchmark tests of new methodologies
- Search for the EDM
- Variation of fundamental constants with time
- Analysis of various experiments
- Study of long-range interactions
- Other nuclear physics applications
- Astrophysics
- Actinide ion studies for chemistry models
- State-insensitive cooling and trapping
- Atomic clocks
- Quantum information



MOTIVATION

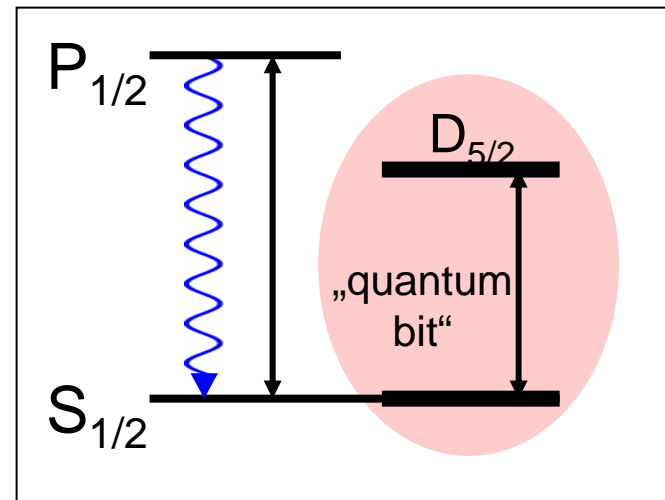
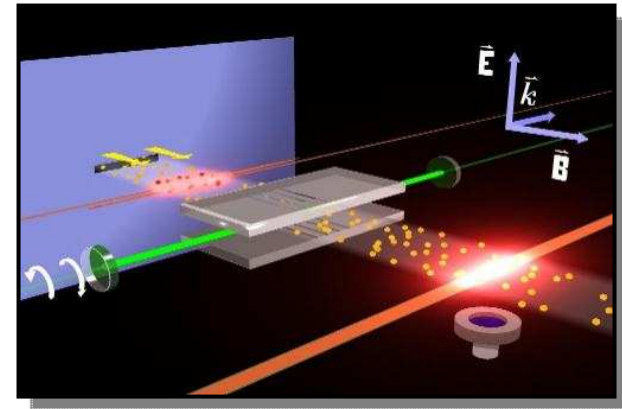


Atomic
Clocks



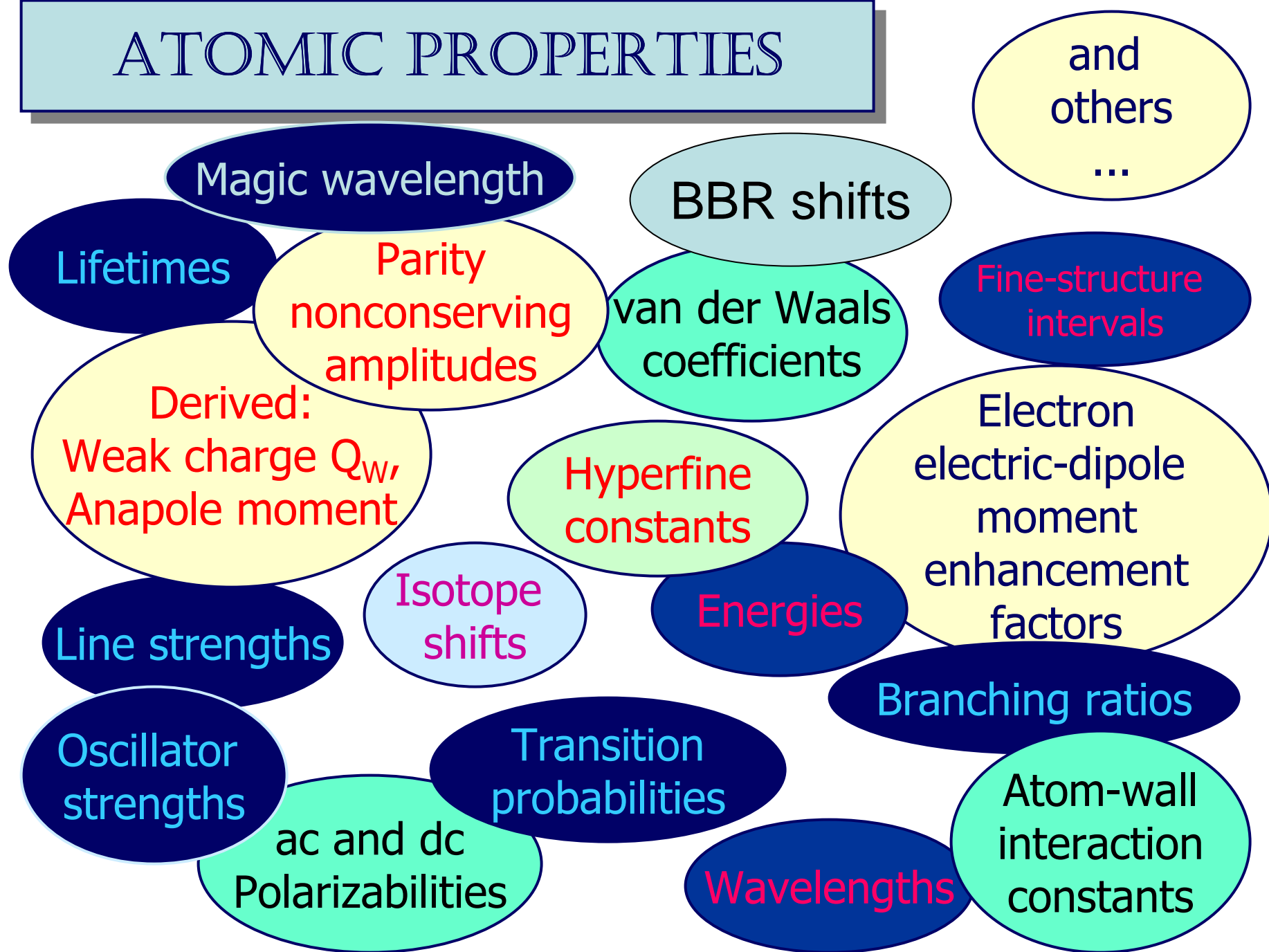
**NEED
ATOMIC
PROPERTIES**

Parity Violation



Quantum information

ATOMIC PROPERTIES



HOW TO ACCURATELY CALCULATE ATOMIC PROPERTIES?

Very precise calculation of atomic properties

WANTED!

We also need to evaluate **uncertainties** of
theoretical values!

EXPERIMENTAL
PNC
STUDIES

PERIODIC TABLE
Atomic Properties of the Elements

NIST

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

EXPERIMENTAL
PNC
STUDIES

- Solids
- Liquids
- Gases
- Artificially Prepared

Physics Laboratory
physics.nist.gov

Standard Reference Data Group
www.nist.gov/srd

Group 1 IA																		Group 2 IIA										Group 13 IIIA										Group 14 IVA										Group 15 VA										Group 16 VIA										Group 17 VIIA										Group 18 VIIIA																																																																																																													
1 H Hydrogen 1.00794 1s 13.5984																												2 He Helium 4.002602 1s 24.5874																																																																																																																																																															
2 Li Lithium 6.941 1s ² 2s 5.3917																		4 Be Beryllium 9.012182 1s ² 2s ² 9.3227																				6 B Boron 10.811 1s ² 2s ² 2p 8.2980										7 C Carbon 12.0107 1s ² 2s ² 2p ² 11.2503										8 N Nitrogen 14.0067 1s ² 2s ² 2p ³ 14.5341										9 O Oxygen 15.9994 1s ² 2s ² 2p ⁴ 13.6181										10 F Fluorine 18.9984032 1s ² 2s ² 2p ⁵ 17.4228										11 Ne Neon 20.1797 1s ² 2s ² 2p ⁶ 15.75645																																																																																																			
3 Na Sodium 22.989770 [Ne]3s 5.1391																		12 Mg Magnesium 24.3050 [Ne]3s ² 7.6462										3 Al Aluminum 26.981538 [Ne]3s ² 3p 5.9858										14 Si Silicon 28.0855 [Ne]3s ² 3p ² 8.1517										15 P Phosphorus 30.973761 [Ne]3s ² 3p ³ 10.4867										16 S Sulfur 32.065 [Ne]3s ² 3p ⁴ 10.3600										17 Cl Chlorine 35.453 [Ne]3s ² 3p ⁵ 12.9675										18 Ar Argon 39.948 [Ne]3s ² 3p ⁶ 15.7596																																																																																																													
4 K Potassium 39.0983 [Ar]4s 4.3407																		20 Ca Calcium 40.078 [Ar]4s 6.1132										21 Sc Scandium 44.955910 [Ar]3d ¹ 4s 6.5615										22 Ti Titanium 47.867 [Ar]3d ² 4s 6.8281										23 V Vanadium 50.9415 [Ar]3d ³ 4s 6.7462										24 Cr Chromium 51.9961 [Ar]3d ⁵ 4s 6.7665										25 Mn Manganese 54.938049 [Ar]3d ⁵ 4s 7.4340										26 Fe Iron 55.845 [Ar]3d ⁶ 4s 7.9024										27 Co Cobalt 58.933200 [Ar]3d ⁷ 4s 7.8810										28 Ni Nickel 58.6934 [Ar]3d ⁸ 4s 7.6398										29 Cu Copper 63.546 [Ar]3d ¹⁰ 4s 7.7264										30 Zn Zinc 65.409 [Ar]3d ¹⁰ 4s 9.3942										31 Ga Gallium 69.723 [Ar]3d ¹⁰ 4s ¹ 4p 5.9993										32 Ge Germanium 72.64 [Ar]3d ¹⁰ 4s ² 4p ² 7.8994										33 As Arsenic 74.92160 [Ar]3d ¹⁰ 4s ² 4p ³ 9.7886										34 Se Selenium 78.96 [Ar]3d ¹⁰ 4s ² 4p ⁴ 9.7524										35 Br Bromine 79.904 [Ar]3d ¹⁰ 4s ² 4p ⁵ 11.8138										36 Kr Krypton 83.798 [Ar]3d ¹⁰ 4s ² 4p ⁶ 13.9996									
5 Rb Rubidium 85.4678 [Kr]5s 4.1771																		38 Sr Strontium 87.62 [Kr]5s 5.6949										39 Y Yttrium 88.90585 [Kr]4d ¹ 5s 6.2173										40 Zr Zirconium 91.224 [Kr]4d ² 5s 6.6339										41 Nb Niobium 92.90638 [Kr]4d ⁴ 5s 6.7589										42 Mo Molybdenum 95.94 [Kr]4d ⁵ 5s 7.0924										43 Tc Technetium (98) [Kr]4d ⁵ 5s 7.28										44 Ru Ruthenium 101.07 [Kr]4d ⁷ 5s 7.3605										45 Rh Rhodium 102.90550 [Kr]4d ⁸ 5s 7.4589										46 Pd Palladium 106.42 [Kr]4d ¹⁰ 8.3369										47 Ag Silver 107.8682 [Kr]4d ¹⁰ 5s 7.5762										48 Cd Cadmium 112.411 [Kr]4d ¹⁰ 5s 8.9938										49 In Indium 114.818 [Kr]4d ¹⁰ 5s ² 5p 7.2964										50 Sn Tin 118.710 [Kr]4d ¹⁰ 5s ² 5p ² 7.2420										51 Sb Antimony 121.760 [Kr]4d ¹⁰ 5s ² 5p ³ 8.6084										52 Te Tellurium 127.60 [Kr]4d ¹⁰ 5s ² 5p ⁴ 9.0095										53 I Iodine 126.90447 [Kr]4d ¹⁰ 5s ² 5p ⁵ 10.4513										54 Xe Xenon 131.293 [Kr]4d ¹⁰ 5s ² 5p ⁶ 12.1298									
6 Cs Cesium 132.90545 [Xe]6s																		86 Ba Barium 137.327 [Xe]6s										72 Hf Hafnium 178.49 [Xe]4f ¹⁴ 5d ² 6s 6.8251										73 Ta Tantalum 180.9479 [Xe]4f ¹⁴ 5d ³ 6s 7.5495										74 W Tungsten 183.84 [Xe]4f ¹⁴ 5d ⁴ 6s 7.8640										75 Re Rhenium 186.207 [Xe]4f ¹⁴ 5d ⁵ 6s 7.8335										76 Os Osmium 190.23 [Xe]4f ¹⁴ 5d ⁶ 6s 8.4382										77 Ir Iridium 192.217 [Xe]4f ¹⁴ 5d ⁷ 6s 8.9588										78 Pt Platinum 195.078 [Xe]4f ¹⁴ 5d ⁹ 6s 8.9588										79 Au Gold 196.96655 [Xe]4f ¹⁴ 5d ¹⁰ 6s 9.2255										80 Hg Mercury 200.59 [Xe]4f ¹⁴ 5d ¹⁰ 6s 10.4375										81 Tl Thallium 204.3833 [Hg]6p 6.1082										82 Pb Lead 207.2 [Hg]6p 7.4167										83 Bi Bismuth 208.98038 [Hg]6p 7.2855										84 Po Polonium (209) [Hg]6p 8.414										85 At Astatine (210) [Hg]6p 8.414										86 Rn Radon (222) [Hg]6p 10.7485																			
7 Fr Francium (223) [Rn]7s																		88 Ra Radium (226) [Rn]7s										104 Rf Rutherfordium (261) [Rn]5f ¹⁴ 6d ² 7s 6.0 ?										105 Db Dubnium (262) [Rn]5f ¹⁴ 6d ³ 7s 6.0 ?										106 Sg Seaborgium (266) [Rn]5f ¹⁴ 6d ⁴ 7s 6.0 ?										107 Bh Bohrium (264) [Rn]5f ¹⁴ 6d ⁵ 7s 6.0 ?										108 Hs Hassium (277) [Rn]5f ¹⁴ 6d ⁶ 7s 6.0 ?										109 Mt Meitnerium (268) [Rn]5f ¹⁴ 6d ⁷ 7s 6.0 ?										110 Uun Ununnilium (281) [Rn]5f ¹⁴ 6d ⁸ 7s 6.0 ?										111 Uuu Unununium (272) [Rn]5f ¹⁴ 6d ⁹ 7s 6.0 ?										112 Uub Ununbium (285) [Rn]5f ¹⁴ 6d ¹⁰ 7s 6.0 ?										114 Uuq Ununquadium (289) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p 6.0 ?										116 Uuh Ununhexium (292) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ² 6.0 ?																																																											
Lanthanides																		57 La Lanthanum 138.9055 [Xe]5d ¹ 6s 5.5769										58 Ce Cerium 140.116 [Xe]4f ¹ 5d ¹ 6s 5.5387										59 Pr Praseodymium 140.90765 [Xe]4f ³ 6s 5.473										60 Nd Neodymium 144.24 [Xe]4f ⁴ 6s 5.5290										61 Pm Promethium (145) [Xe]4f ⁵ 6s 5.582										62 Sm Samarium 150.36 [Xe]4f ⁶ 6s 5.6437										63 Eu Europium 151.964 [Xe]4f ⁷ 6s 5.6704										64 Gd Gadolinium 157.25 [Xe]4f ⁷ 5d ¹ 6s 6.1498										65 Tb Terbium 158.92534 [Xe]4f ⁹ 6s 5.8538										66 Dy Dysprosium 162.500 [Xe]4f ¹⁰ 6s 5.9389										67 Ho Holmium 164.93032 [Xe]4f ¹¹ 6s 6.0215										68 Er Erbium 167.259 [Xe]4f ¹² 6s 6.1077										69 Tm Thulium 168.93421 [Xe]4f ¹³ 6s 6.1843										70 Yb Ytterbium 173.04 [Xe]4f ¹⁴ 6s 6.2542										71 Lu Lutetium 174.967 [Xe]4f ¹⁴ 5d ¹ 6s 5.4259																													
Actinides																		89 Ac Actinium (227) [Rn]6d ¹ 7s 5.17										90 Th Thorium 232.0381 [Rn]6d ² 7s 6.3067										91 Pa Protactinium 231.03688 [Rn]5f ² 6d ¹ 7s 5.89										92 U Uranium 238.02891 [Rn]5f ³ 6d ¹ 7s 6.1941										93 Np Neptunium (237) [Rn]5f ⁴ 6d ¹ 7s 6.2657										94 Pu Plutonium (244) [Rn]5f ⁶ 7s 6.0260										95 Am Americium (243) [Rn]5f ⁷ 7s 5.9738										96 Cm Curium (247) [Rn]5f ⁸ 6d ¹ 7s 5.9914										97 Bk Berkelium (247) [Rn]5f ⁹ 7s 6.1979										98 Cf Californium (251) [Rn]5f ¹⁰ 7s 6.2817										99 Es Einsteinium (252) [Rn]5f ¹¹ 7s 6.42										100 Fm Fermium (257) [Rn]5f ¹² 7s 6.50										101 Md Mendelevium (258) [Rn]5f ¹³ 7s 6.58										102 No Nobelium (259) [Rn]5f ¹⁴ 7s 6.65										103 Lr Lawrencium (262) [Rn]5f ¹⁴ 7s ² 7p 4.9 ?																													

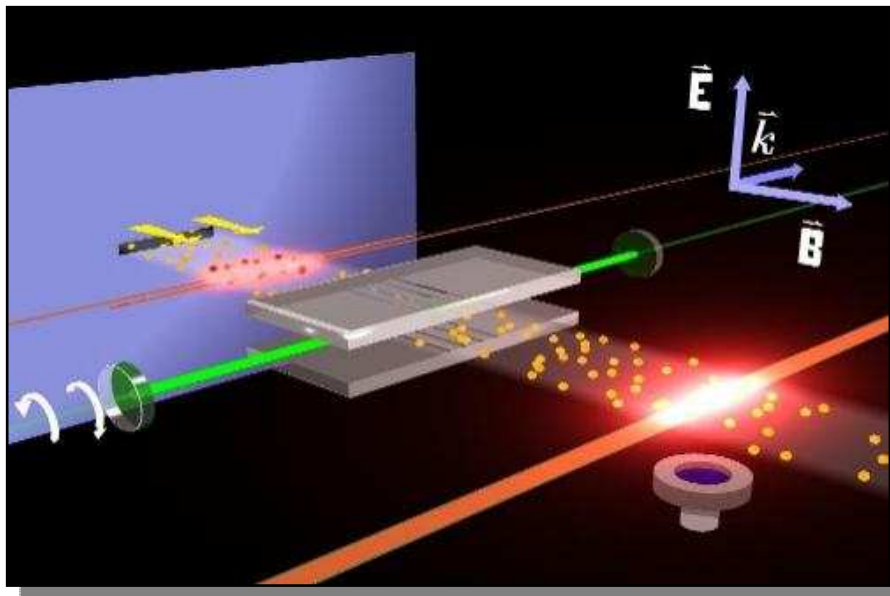
[†]Based upon ¹²C. () indicates the mass number of the most stable isotope.

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

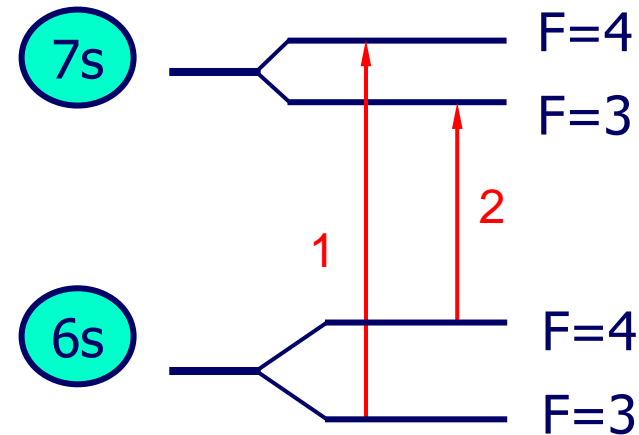
NIST SP 966 (September 2003)

THE MOST PRECISE MEASUREMENT OF PNC AMPLITUDE (IN CESIUM)

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



0.3% accuracy

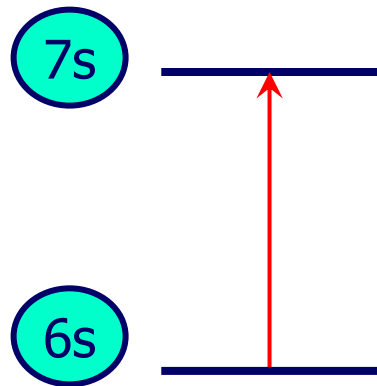


$$\frac{\text{Im}(E_{\text{PNC}})}{\beta} = \begin{cases} -1.6349(80) \text{ mV/cm} & \mathbf{1} \\ -1.5576(77) \text{ mV/cm} & \mathbf{2} \end{cases}$$

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

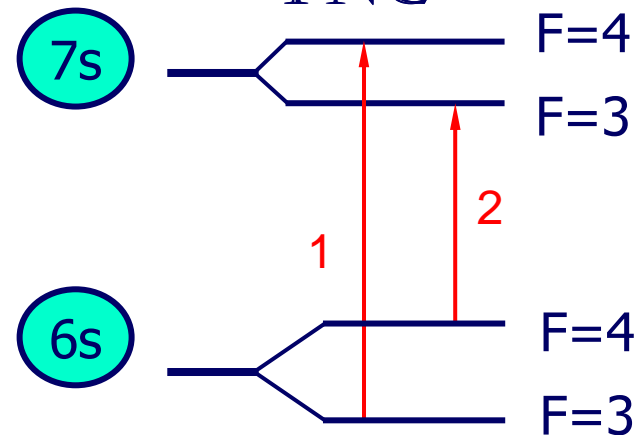


Average of 1 & 2

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

Weak Charge Q_W

NUCLEAR
SPIN-DEPENDENT
PNC



Difference of 1 & 2

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

Nuclear anapole moment

ANALYSIS OF CS PNC EXPERIMENT: THEORY INPUT

Weak Charge Q_W

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

Need theory $E_{\text{PNC}}^{\text{si}}$
calculation in terms
of Q_W

Need β

Nuclear anapole moment

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

Need theory $E_{\text{PNC}}^{\text{sd}}$
calculation in terms
of anapole moment

Need β

CALCULATION OF SPIN-INDEPENDENT PNC AMPLITUDE

Electric-dipole matrix elements

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

Energies

PNC matrix elements

Nuclear density function

$$H_{\text{PNC}} = \frac{G_F}{2\sqrt{2}} Q_W \gamma_5 \rho(r)$$

G_F - Universal Fermi coupling constant

γ_5 - Dirac matrix

VECTOR TRANSITION POLARIZABILITY β

Tensor transition polarizability β can be calculated from electric-dipole matrix elements and corresponding energies.

Theory recommended value [1]: $27.11(22) a_0^3$

80% uncertainty comes from one transition $6s-7p_{3/2}$!

New measurement of 6s-7p matrix elements [2]: $27.22(11) a_0^3$

Measured value (from $M1_{\text{HFS}} / \beta$) [3]: $27.02(8) a_0^3$

[1] M.S.Safronova, W.R. Johnson, and A. Derevianko, PRA 60, 4476 (1999)

[2] A.A. Vasilyev, I.M. Savukov, M.S. Safronova, and H.G. Berry, PRA 66, 020101 (2002)

[3] S.C. Bennett and C.E. Wieman, PRL 82, 2484 (1999)

THEORY: EVALUATION OF THE UNCERTAINTY

HOW TO ESTIMATE WHAT YOU DO NOT KNOW?

I. *Ab initio* calculations in different approximations:

- (a) Evaluation of the size of the correlation corrections
- (b) Importance of the high-order contributions
- (c) Distribution of the correlation correction

II. Semi-empirical scaling: estimate missing terms

HOW TO EVALUATE ACCURACY OF THE THEORETICAL PNC AMPLITUDE?

Indirect method: compare the other atomic properties with experiment.

Direct method: estimate omitted terms and/or do a scatter analysis.

Direct summation method:

- Use semi-empirical scaling to estimate the magnitude of the dominant omitted terms.
- Use different sets of data for energies, dipole, and PNC matrix elements and look at the scatter of the values.

SCATTER ANALYSIS: AN EXAMPLE

Energies	Dipole	PNC	Value
DHF	DHF	DHF	0.735
Expt.	SD	SD	0.894
Expt.	"best values"	SD	0.892
Expt.	SD scaled	SD scaled	0.899
Expt.	"best values"	SD scaled	0.882

Blundell et al. (1992)

Note: Dzuba et al. (2002) uses various energy fits for dominant terms and look at the scatter of the resulting values.

PROBLEMS WITH UNCERTAINTY ANALYSIS

It is the best estimate, not a certain result.
Not all of the missing terms are estimated.
Uncertainties in other (smaller terms) are assumed to be small.
Other smaller (non-Coulomb terms)?

However, it is a best (and rather unique) attempt to actually place a reasonable uncertainty on the theoretical value.

SUMMARY OF THE PNC AMPLITUDE CALCULATIONS

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

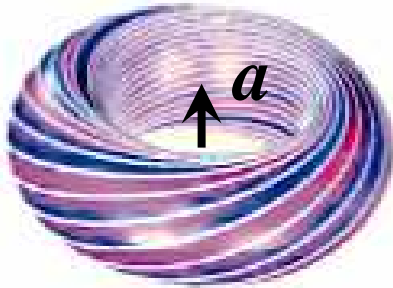
-0.909 Safronova & Johnson (1999)
-0.905 Kozlov et al. (2001)
-0.908 Dzuba et al. (2002) **0.5% uncertainty**

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

DETERMINATION OF Q_W

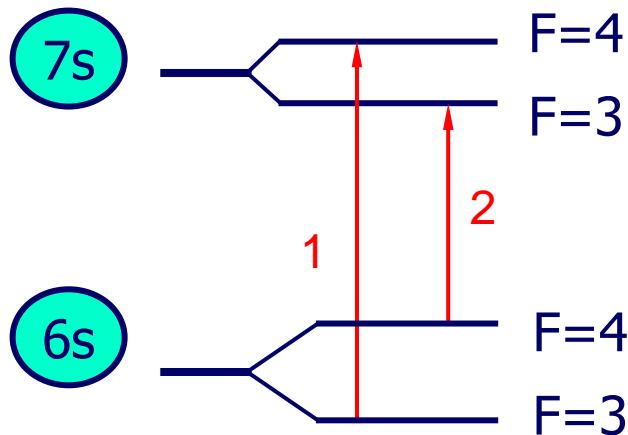
Wood et al. (1997) $\text{Im}(E_{\text{PNC}})/\beta$	-72.11(27) _{expt} (89) _{theor}	1 σ
Bennett & Wieman (1999) Measurement of β	-72.06(28) _{expt} (34) _{theor}	2.5 σ
Derevianko (2000,2002) Calculation of Breit correction	-72.61(28) _{expt} (34/73) _{theor}	1.3 σ /0.7 σ
Dzuba et al. (2000) Calculation of Breit correction	-72.42(28) _{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(28) _{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(28) _{expt} (36) _{th}	0.6 σ

SPIN-DEPENDENT PARITY VIOLATION: NUCLEAR ANAPOLE MOMENT



Parity-violating nuclear moment

Valence nucleon density



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

Anapole moment

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

HOW TO DERIVE THE VALUE OF THE NUCLEAR ANAPOLE MOMENT?

Experimental value

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

Theoretical value
of spin-dependent
PNC amplitude
in terms of K_a

+

Experimental or theoretical value
of vector transition polarizability β

$$\Delta_{34-43}^{\text{expt}} = K \left[\Delta E_{\text{PNC}}^{(\text{sd})} \right]_{34-43}^{\text{theory}} (1/\beta)$$

$K \neq K_a$ More spin-dependent
PNC effects!

MORE SPIN-DEPENDENT PNC EFFECTS

$$\mathcal{K} = \mathcal{K}_a + \mathcal{K}_2 + \mathcal{K}_{\text{hf}}$$

(V_e/A_N)
interaction

Same Hamiltonian as
anapole moment term
with $\mathcal{K}_a \Rightarrow \mathcal{K}_2$

Weak-hyperfine
interference term

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

ANAPOLE MOMENT AND AXIAL-VECTOR TERMS

Electric-dipole matrix elements

$$E_{\text{PNC}}^{(2,a)} = \mathcal{A}_1 \sum_{j \neq v} \frac{\langle w || z || j \rangle \langle j || H_{\text{PNC}}^{(2,a)} || v \rangle}{\epsilon_v - \epsilon_j} + \mathcal{A}_2 \sum_{j \neq w} \frac{\langle w || H_{\text{PNC}}^{(2,a)} || j \rangle \langle j || z || v \rangle}{\epsilon_w - \epsilon_j}$$

PNC matrix elements

Angular momentum coefficients

$$H_{\text{PNC}}^{(2,a)} = \frac{G_F}{\sqrt{2}} \mathbf{K}_i \boldsymbol{\alpha} \boldsymbol{\Pi} \rho_v(r), \quad i = 2, a$$

WEAK-HYPERFINE INTERFERENCE TERM κ_{hf}

$$\begin{aligned}
 \langle w | F M_F | z | v | F I M_I \rangle^{(hf)} = & \quad \text{Hyperfine} \quad \text{Spin-independent PNC} \\
 & \quad \quad \quad \swarrow \quad \quad \downarrow \quad \quad \searrow \text{E1} \\
 \sum_{\substack{m \neq w \\ n \neq w}} \frac{\langle w | H^{(1)} | n \rangle \langle n | H^{(hf)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)(E_w - E_n)} + \sum_{\substack{m \neq w \\ n \neq w}} \frac{\langle w | H^{(hf)} | n \rangle \langle n | H^{(1)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)(E_w - E_n)} \\
 + \sum_{\substack{m \neq w \\ n \neq v}} \frac{\langle w | H^{(1)} | m \rangle \langle m | z | n \rangle \langle n | H^{(hf)} | v \rangle}{(E_w - E_m)(E_v - E_n)} + \sum_{\substack{m \neq w \\ n \neq v}} \frac{\langle w | H^{(hf)} | m \rangle \langle m | z | n \rangle \langle n | H^{(1)} | v \rangle}{(E_w - E_m)(E_v - E_n)} \\
 + \sum_{\substack{m \neq v \\ n \neq v}} \frac{\langle w | z | n \rangle \langle n | H^{(1)} | m \rangle \langle m | H^{(hf)} | v \rangle}{(E_v - E_m)(E_v - E_n)} + \sum_{\substack{m \neq v \\ n \neq v}} \frac{\langle w | z | n \rangle \langle n | H^{(hf)} | m \rangle \langle m | H^{(1)} | v \rangle}{(E_v - E_m)(E_v - E_n)} \\
 - \langle w | H^{(hf)} | w \rangle \sum_{m \neq w} \frac{\langle w | H^{(1)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)^2} - \sum_{n \neq v} \frac{\langle w | z | n \rangle \langle n | H^{(1)} | v \rangle}{(E_v - E_n)^2} \langle v | H^{(hf)} | v \rangle,
 \end{aligned}$$

NUCLEAR ANAPOLE MOMENT: SUMMARY

Group	\mathcal{K}	\mathcal{K}_2	\mathcal{K}_{hf}	\mathcal{K}_a
Johnson et al. [1]	0.117(16)	0.0140	0.0049	0.098(16)
Haxton et al. [2]	0.112(16)	0.0140	0.0078	0.090(16)
Flambaum and Murray [3]	0.112(16)	0.0111	0.0071	0.092(16)
Bouchiat and Piketty [4]		0.0084	0.0078	

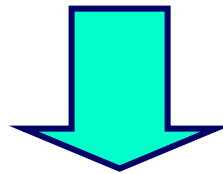
- [1] W.R. Johnson, M.S. Safronova and U.I. Safronova, Phys. Rev. A 67, 062106 (2003)
[2] W. C. Haxton, C.-P. Liu, and M. J. Ramsey-Musolf, Phys. Rev. Lett. 86, 5247 (2001)
[3] V. V. Flambaum and D. W. Murray, Phys. Rev. C 56, 1641 (1997)
[4] C. Bouchiat and C. A. Piketty, Phys. Lett. B 269, 195 (1991)

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?

NEW (ALL-ORDER) CALCULATION OF SPIN-DEPENDENT PNC

Electric-dipole matrix elements

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

PNC matrix elements

Fist four terms in the sums are replaced by
all-order matrix elements
Same accuracy is expected as spin-independent PNC

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.

All-order calculation of spin-dependent PNC amplitude:

$$\kappa = 0.110(16)^*$$

No significant difference with RPA value $\kappa = 0.117(16)$ is found.

NEED NEW EXPERIMENTS!!!

*M.S. Safronova, E. Iskrenova-Tchoukova, and W.R. Johnson,
to be submitted to Phys. Rev. Lett.

THEORY:
HOW TO CALCULATE
PNC AND DIPOLE
MATRIX ELEMENTS?

PERIODIC TABLE
Atomic Properties of the Elements

NIST

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

EXPERIMENTAL
PNC
STUDIES

- █ Solids
- █ Liquids
- █ Gases
- █ Artificially Prepared

Physics Laboratory
physics.nist.gov

Standard Reference Data Group
www.nist.gov/srd

Group 1 IA	2 IIA	EXPERIMENTAL PNC STUDIES										13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA											
1 H Hydrogen 1.00794 $1s^1$ 13.5984												B Boron 10.811 $1s^2 2s^2 2p^1$ 8.2980	C Carbon 12.0107 $1s^2 2s^2 2p^2$ 11.2503	N Nitrogen 14.0067 $1s^2 2s^2 2p^3$ 14.5341	O Oxygen 15.9994 $1s^2 2s^2 2p^4$ 13.6181	F Fluorine 18.9984032 $1s^2 2s^2 2p^5$ 17.4228	Ne Neon 20.1797 $1s^2 2s^2 2p^6$ 21.5645											
2 Li Lithium 6.941 $1s^2 2s^1$ 5.3917	Be Beryllium 9.012182 $1s^2 2s^2$ 9.3227										Al Aluminum 26.981538 $[Ne]3s^2 3p^1$ 5.9858	Si Silicon 28.0855 $[Ne]3s^2 3p^2$ 8.1517	P Phosphorus 30.973761 $[Ne]3s^2 3p^3$ 10.4867	S Sulfur 32.065 $[Ne]3s^2 3p^4$ 10.3600	Cl Chlorine 35.453 $[Ne]3s^2 3p^5$ 12.9675	Ar Argon 39.948 $[Ne]3s^2 3p^6$ 15.7596												
3 Na Sodium 22.989770 $[Ne]3s^1$ 5.1391	Mg Magnesium 24.3050 $[Ne]3s^2$ 7.6462										K Potassium 39.0983 $[Ar]4s^1$ 4.3407	Ca Calcium 40.078 $[Ar]4s^2$ 6.1132	Sc Scandium 44.955910 $[Ar]3d^1 4s^2$ 6.5615	Ti Titanium 47.867 $[Ar]3d^2 4s^2$ 6.8281	V Vanadium 50.9415 $[Ar]3d^3 4s^2$ 6.7462	Cr Chromium 51.9961 $[Ar]3d^5 4s^1$ 6.7665	Mn Manganese 54.938049 $[Ar]3d^5 4s^2$ 7.4340	Fe Iron 55.845 $[Ar]3d^6 4s^2$ 7.9024	Co Cobalt 58.933200 $[Ar]3d^7 4s^2$ 7.8810	Ni Nickel 58.6934 $[Ar]3d^8 4s^2$ 7.6398	Cu Copper 63.546 $[Ar]3d^9 4s^1$ 7.7264	Zn Zinc 65.409 $[Ar]3d^10 4s^1$ 9.3942	Ga Gallium 69.723 $[Ar]3d^10 4s^2 4p^1$ 5.9993	Ge Germanium 72.64 $[Ar]3d^10 4s^2 4p^2$ 7.8994	As Arsenic 74.92160 $[Ar]3d^10 4s^2 4p^3$ 9.7886	Se Selenium 78.96 $[Ar]3d^10 4s^2 4p^4$ 9.7524	Br Bromine 79.904 $[Ar]3d^10 4s^2 4p^5$ 11.8138	Kr Krypton 83.798 $[Ar]3d^10 4s^2 4p^6$ 13.9996
4 K Potassium 39.0983 $[Ar]4s^1$ 4.3407	Ca Calcium 40.078 $[Ar]4s^2$ 6.1132	Sc Scandium 44.955910 $[Ar]3d^1 4s^2$ 6.5615	Ti Titanium 47.867 $[Ar]3d^2 4s^2$ 6.8281	V Vanadium 50.9415 $[Ar]3d^3 4s^2$ 6.7462	Cr Chromium 51.9961 $[Ar]3d^5 4s^1$ 6.7665	Mn Manganese 54.938049 $[Ar]3d^5 4s^2$ 7.4340	Fe Iron 55.845 $[Ar]3d^6 4s^2$ 7.9024	Co Cobalt 58.933200 $[Ar]3d^7 4s^2$ 7.8810	Ni Nickel 58.6934 $[Ar]3d^8 4s^2$ 7.6398	Cu Copper 63.546 $[Ar]3d^9 4s^1$ 7.7264	Zn Zinc 65.409 $[Ar]3d^10 4s^1$ 9.3942	Ga Gallium 69.723 $[Ar]3d^10 4s^2 4p^1$ 5.9993	Ge Germanium 72.64 $[Ar]3d^10 4s^2 4p^2$ 7.8994	As Arsenic 74.92160 $[Ar]3d^10 4s^2 4p^3$ 9.7886	Se Selenium 78.96 $[Ar]3d^10 4s^2 4p^4$ 9.7524	Br Bromine 79.904 $[Ar]3d^10 4s^2 4p^5$ 11.8138	Kr Krypton 83.798 $[Ar]3d^10 4s^2 4p^6$ 13.9996											
5 Rb Rubidium 85.4678 $[Kr]5s^1$ 4.1771	Sr Strontium 87.62 $[Kr]5s^2$ 5.6915	Y Yttrium 88.90585 $[Kr]4d^1 5s^2$ 6.2173	Zr Zirconium 91.224 $[Kr]4d^2 5s^2$ 6.6339	Nb Niobium 92.90638 $[Kr]4d^4 5s^1$ 6.7589	Mo Molybdenum 95.94 $[Kr]4d^5 5s^1$ 7.0924	Tc Technetium (98) $[Kr]4d^5 5s^2$ 7.28	Ru Ruthenium 101.07 $[Kr]4d^7 5s^1$ 7.3605	Rh Rhodium 102.90550 $[Kr]4d^8 5s^1$ 7.4589	Pd Palladium 106.42 $[Kr]4d^10$ 8.3369	Ag Silver 107.8682 $[Kr]4d^9 5s^1$ 7.5762	Cd Cadmium 112.411 $[Kr]4d^10 5s^2$ 8.9938	In Indium 114.818 $[Kr]4d^10 5s^2 5p^1$ 7.2964	Sn Tin 118.710 $[Kr]4d^10 5s^2 5p^2$ 7.2420	Sb Antimony 121.760 $[Kr]4d^10 5s^2 5p^3$ 8.6084	Te Tellurium 127.60 $[Kr]4d^10 5s^2 5p^4$ 9.0095	I Iodine 126.90447 $[Kr]4d^10 5s^2 5p^5$ 10.4513	Xe Xenon 131.293 $[Kr]4d^10 5s^2 5p^6$ 12.1298											
6 Cs Cesium 132.90545 $[Xe]6s^1$	Ba Barium 137.327 $[Xe]6s^2$										Tl Thallium 204.3833 $[Hg]6p^1$ 6.1082	Pb Lead 207.2 $[Hg]6p^2$ 7.4167	Bi Bismuth 208.98038 $[Hg]6p^3$ 7.2855	Po Polonium (209) $[At]6p^4$	At Astatine (210) $[Hg]6p^5$	Rn Radon (222) $[Hg]6p^6$ 10.7485												
7 Fr Francium (223) $[Rn]7s^1$ 4.0727	Ra Radium (226) $[Rn]7s^2$ 5.278										Rf Rutherfordium (261) $[Rn]5f^14 6d^2 7s^2$ 6.0 ?	Db Dubnium (262)	Sg Seaborgium (266)	Bh Bohrium (264)	Hs Hassium (277)	Mt Meitnerium (268)	Uun Ununnilium (271)	Uuu Ununquadium (273)	Uub Ununseptium (275)	Uuq Ununquadium (289)	Uuh Ununhexium (292)							
		Lanthanides																										
		Actinides																										
			La Lanthanum 138.9055 $[Xe]5d^1 6s^2$ 5.5769	Ce Cerium 140.116 $[Xe]4f^1 5d^1 6s^2$ 5.5387	Pr Praseodymium 140.90765 $[Xe]4f^3 6s^2$ 5.473	Nd Neodymium 144.24 $[Xe]4f^4 6s^2$ 5.5250	Pm Promethium (145) $[Xe]4f^5 6s^2$ 5.58	Sm Samarium 150.36 $[Xe]4f^6 6s^2$ 5.6437	Eu Europium 151.964 $[Xe]4f^7 6s^2$ 5.6704	Gd Gadolinium 157.25 $[Xe]4f^7 5d^1 6s^2$ 6.1498	Tb Terbium 158.92534 $[Xe]4f^9 6s^2$ 5.8538	Dy Dysprosium 162.500 $[Xe]4f^10 6s^2$ 5.9389	Ho Holmium 164.93032 $[Xe]4f^11 6s^2$ 6.215	Er Erbium 167.259 $[Xe]4f^12 6s^2$ 6.1077	Tm Thulium 168.934 $[Xe]4f^13 6s^2$ 6.1843	Yb Ytterbium 173.04 $[Xe]4f^14 6s^2$ 6.2542	Lu Lutetium 174.967 $[Xe]4f^14 5d^1 6s^2$ 6.4259											
			Ac Actinium (227) $[Rn]5f^7 6d^1 7s^2$ 5.17	Th Thorium 232.0381 $[Rn]6d^2 7s^2$ 6.3067	Pa Protactinium 231.03688 $[Rn]5f^2 6d^1 7s^2$ 5.89	U Uranium 238.02891 $[Rn]5f^3 6d^1 7s^2$ 6.1941	Np Neptunium (237) $[Rn]5f^4 6d^1 7s^2$ 6.2657	Pl Plutonium (244) $[Rn]5f^6 7s^2$ 6.0260	Am Americium (243) $[Rn]5f^7 7s^2$ 5.9738	Cm Curium (247) $[Rn]5f^7 6d^1 7s^2$ 5.9914	Bk Berkelium (247) $[Rn]5f^9 7s^2$ 6.1979	Cf Californium (251) $[Rn]5f^10 7s^2$ 6.2817	Es Einsteinium (252) $[Rn]5f^11 7s^2$ 6.42	Fm Fermium (257) $[Rn]5f^12 7s^2$ 6.50	Md Mendelevium (258) $[Rn]5f^13 7s^2$ 6.58	No Nobelium (259) $[Rn]5f^14 7s^2$ 6.65	Lr Lawrencium (262) $[Rn]5f^14 7s^2 7p^1$ 4.9 ?											

[†]Based upon ¹²C. () 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)

SUMMARY OF THEORY METHODS

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

- Configuration interaction + second-order MBPT
- Configuration interaction + all-order methods*

*under development

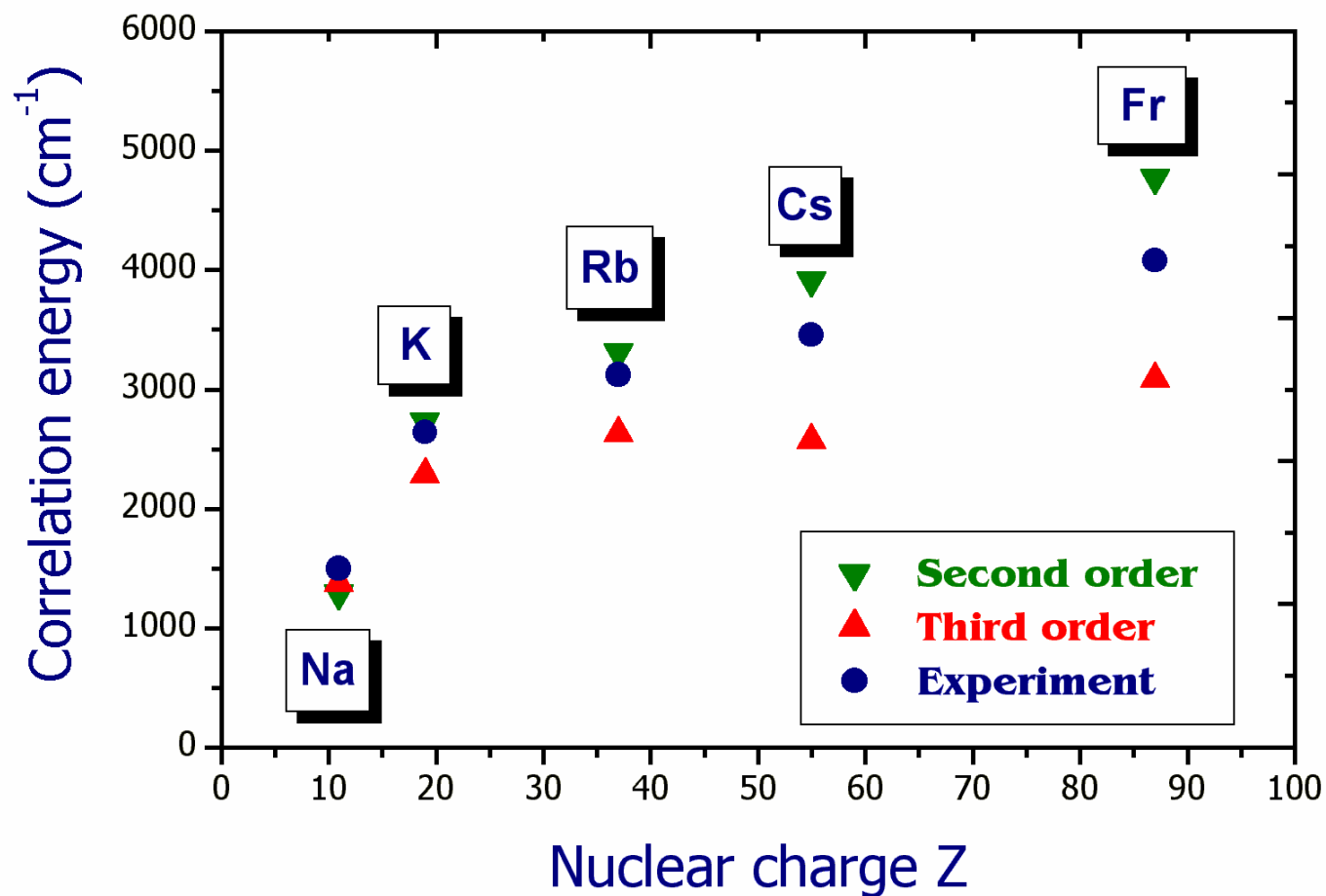
SUMMARY OF THEORY METHODS

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

- Configuration interaction + second-order MBPT
- Configuration interaction + all-order methods*

*under development

Perturbation theory: Correlation correction to ground state energies of alkali-metal atoms



PERIODIC TABLE
Atomic Properties of the Elements

NIST

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

RELATIVISTIC
ALL-ORDER
METHOD

- Solids
- Liquids
- Gases
- Artificially Prepared

Group	1	2											13	14	15	16	17	18
IA	IIA												IIIA	IVA	VA	VIA	VIIA	VIIIA
1	H Hydrogen 1.00794												B Boron 10.811	C Carbon 12.0107	N Nitrogen 14.0067	O Oxygen 15.9994	F Fluorine 18.9984032	Ne Neon 20.1797
2	Li Lithium 6.941	Be Beryllium 9.012182											Al Aluminum 26.981538	Si Silicon 28.0855	P Phosphorus 30.973761	S Sulfur 32.065	Cl Chlorine 35.453	Ar Argon 39.948
3	Na Sodium 22.989770	Mg Magnesium 24.3050											Ga Gallium 69.723	Ge Germanium 72.64	As Arsenic 74.92160	Se Selenium 78.96	Br Bromine 79.904	Kr Krypton 83.798
4	K Potassium 39.0983	Ca Calcium 40.078	Sc Scandium 44.955910	Ti Titanium 47.867	V Vanadium 50.9415	Cr Chromium 51.9961	Mn Manganese 54.938049	Fe Iron 55.845	Co Cobalt 58.933200	Ni Nickel 58.6934	Cu Copper 63.546	Zn Zinc 65.409	Ga Gallium 69.723	Ge Germanium 72.64	As Arsenic 74.92160	Se Selenium 78.96	Br Bromine 79.904	Kr Krypton 83.798
5	Rb Rubidium 85.4678	Sr Strontium 87.62	Y Yttrium 88.90585	Zr Zirconium 91.224	Nb Niobium 92.90638	Mo Molybdenum 95.94	Tc Technetium (98)	Ru Ruthenium 101.07	Rh Rhodium 102.90550	Pd Palladium 106.42	Ag Silver 107.8682	Cd Cadmium 112.411	In Indium 114.818	Sn Tin 118.710	Sb Antimony 121.760	Te Tellurium 127.60	I Iodine 126.90447	Xe Xenon 131.293
6	Cs Cesium 132.90545	Ba Barium 137.327		Hf Hafnium 178.49	Ta Tantalum 180.9479	W Tungsten 183.84	Re Rhenium 186.207	Os Osmium 190.23	Ir Iridium 192.217	Pt Platinum 195.078	Au Gold 196.96655	Hg Mercury 200.59	Tl Thallium 204.3833	Pb Lead 207.2	Bi Bismuth 208.98038	Po Polonium (209)	At Astatine (210)	Rn Radon (222)
7	Fr Francium (223)	Ra Radium (226)		Rf Rutherfordium (261)	Db Dubnium (262)	Sg Seaborgium (266)	Bh Bohrium (264)	Hs Hassium (277)	Mt Meitnerium (268)	Uun Ununilium (271)	Uuq Ununquadium (272)	Uub Ununbium (285)		Uuq Ununquadium (289)		Uuh Ununhexium (282)		
			Ac Actinium (227)	Th Thorium 232.0381	Pa Protactinium 231.03688	U Uranium 238.02891	Np Neptunium (237)	Pu Plutonium (244)	Am Americium (243)	Cm Curium (247)	Bk Berkelium (247)	Cf Californium (251)	Es Einsteinium (252)	Fm Fermium (257)	Md Mendelevium (258)	No Nobelium (259)	Lr Lawrencium (262)	

Singly-ionized ions

Atomic Number: 58
Ground-state Level: $1G_4$
Symbol: **Ce**
Name: Cerium
Atomic Weight: 140.116
Ground-state Configuration: $[Xe]4f5d6s^2$
Ionization Energy (eV): 5.5387

[†]Based upon ¹²C. () indicates the mass number of the most stable isotope.

RELATIVISTIC ALL-ORDER METHOD

Sum over infinite sets of **many-body perturbation theory** (MBPT) terms.

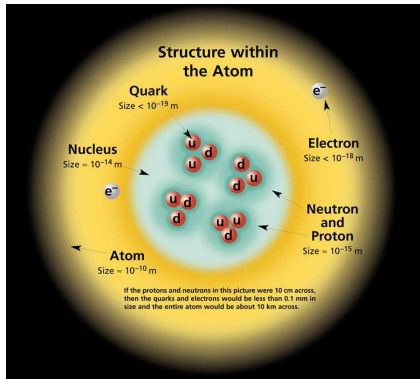
Scheme:

Calculate the atomic wave functions and energies

Calculate various matrix elements

Calculate “derived” properties
such as PNC amplitudes

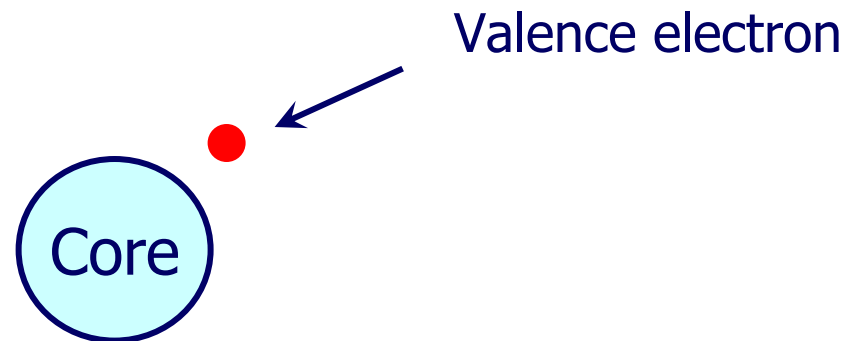
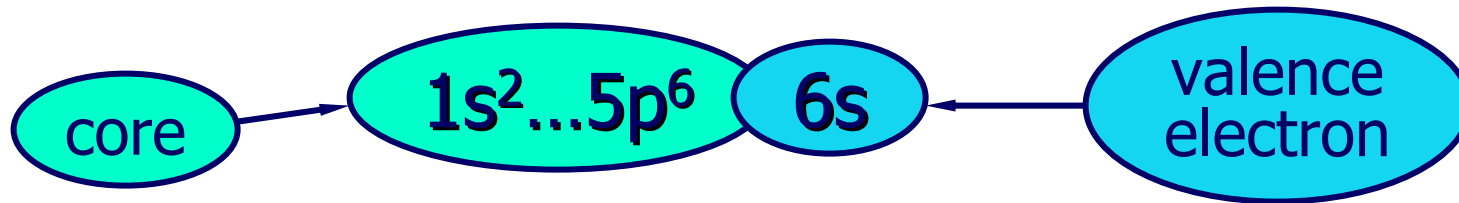




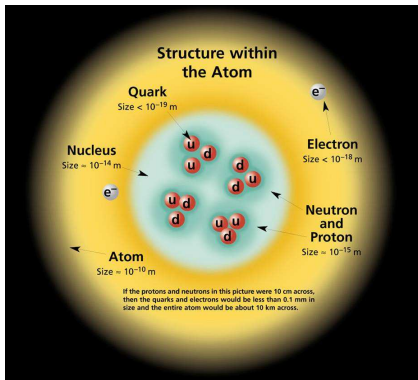
LOWEST ORDER

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

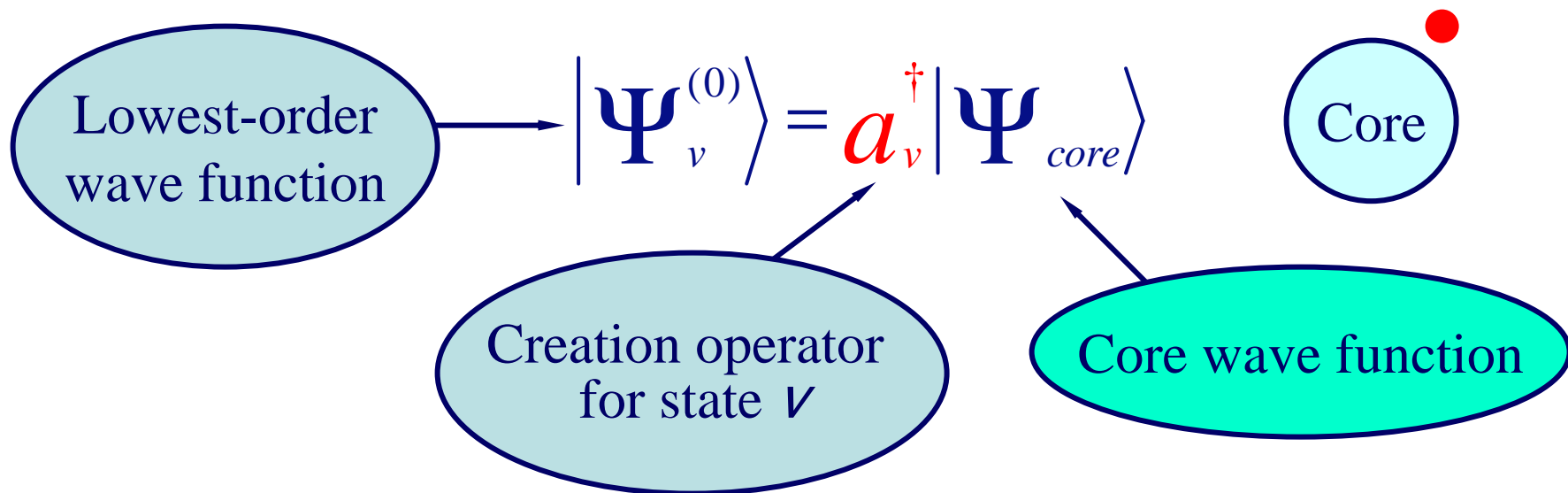
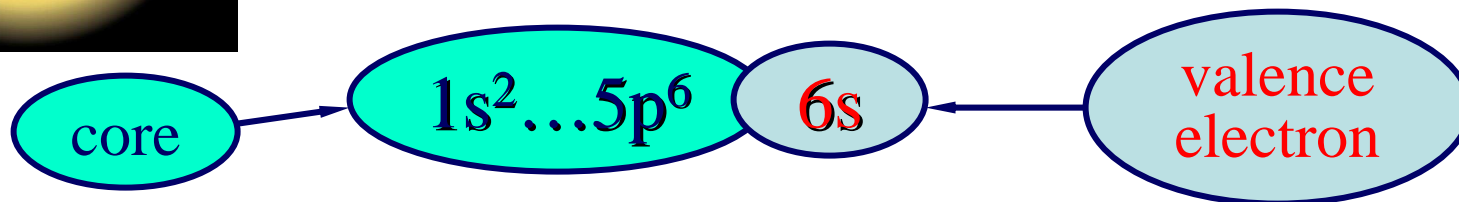
Cs $Z=55$



LOWEST-ORDER ATOMIC WAVE FUNCTION

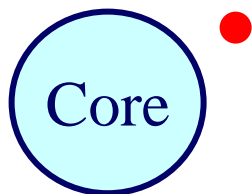


Cs: atom with single (valence) electron outside of a closed core.



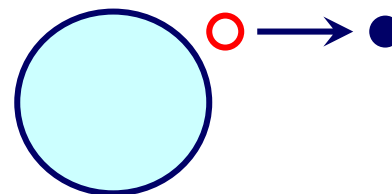
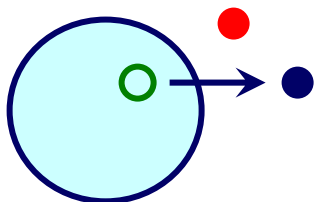
ALL-ORDER ATOMIC WAVE FUNCTION (SD)

Lowest order

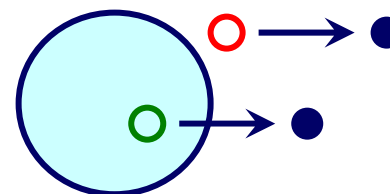
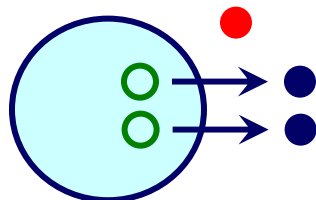


- core
- valence electron
- any excited orbital

Single-particle excitations

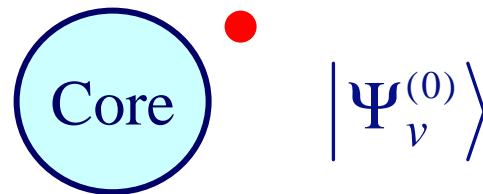


Double-particle excitations



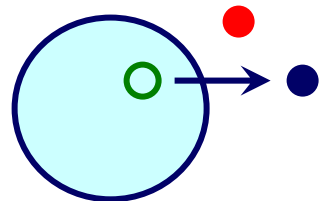
ALL-ORDER ATOMIC WAVE FUNCTION (SD)

Lowest order

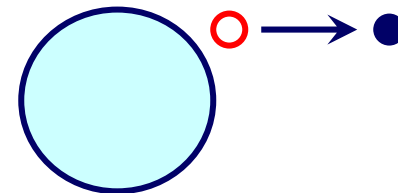


- core
- valence electron
- any excited orbital

Single-particle
excitations

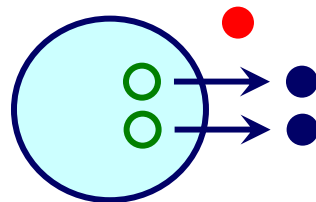


$$\sum_{ma} \rho_{ma} a_m^\dagger a_a |\Psi_v^{(0)}\rangle$$

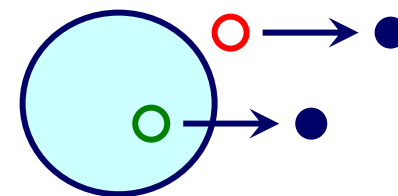


$$\sum_{m \neq v} \rho_{mv} a_m^\dagger a_v |\Psi_v^{(0)}\rangle$$

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 of equations!

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!

Memory & storage of ρ_{mnab} : it is a **really large** file!

Actual implementation: Problem 2

These are really complicated equations !!!

- “Quadruple” term:

$$\sum_{rs} g_{mnr s} \rho_{rsab}$$

a, b core
(17 shells)

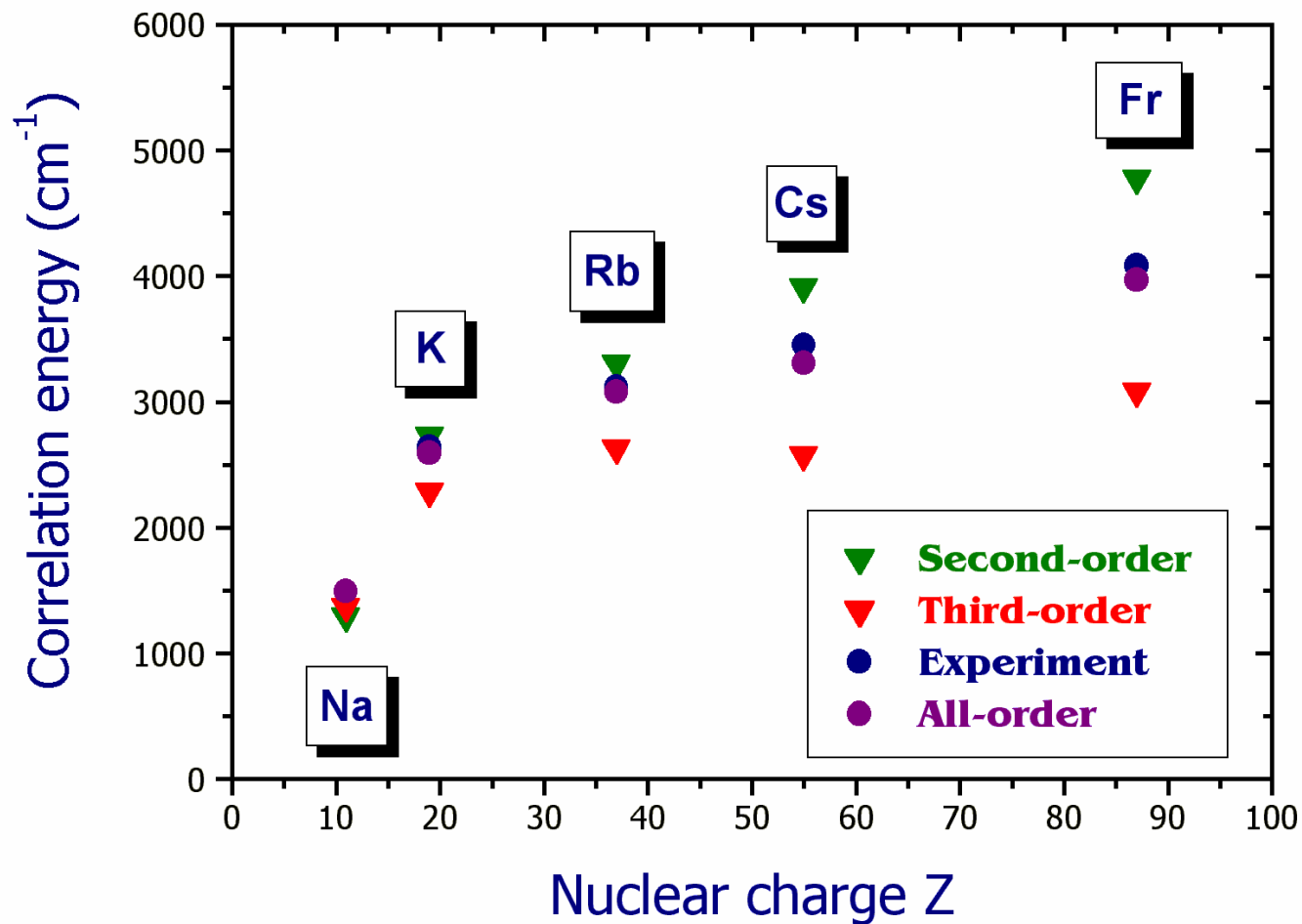
Indices *mnr s* can be **ANY** orbitals

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

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

- Program has to be exceptionally efficient!

All-order method: Correlation correction to ground state energies of alkali-metal atoms



ALL-ORDER MATRIX ELEMENTS

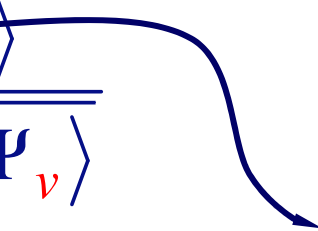
So we calculated all ρ_{ma} , ρ_{mnab} , ρ_{mv} , ρ_{mnva} .

We now have a really large file with ρ .

How do we calculate E1 and PNC matrix elements?

$$Z_{wv}^{PNC} = \frac{\langle \Psi_w | H_{PNC} | \Psi_v \rangle}{\sqrt{\langle \Psi_w | \Psi_w \rangle \langle \Psi_v | \Psi_v \rangle}}$$

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



RESULTS FOR ALKALI-METAL ATOMS: E1 MATRIX ELEMENTS

	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. Schmoranzer, 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)

EXTENSIONS OF THE ALL ORDER METHOD

Add more terms to the all order wave-function

Non-linear terms

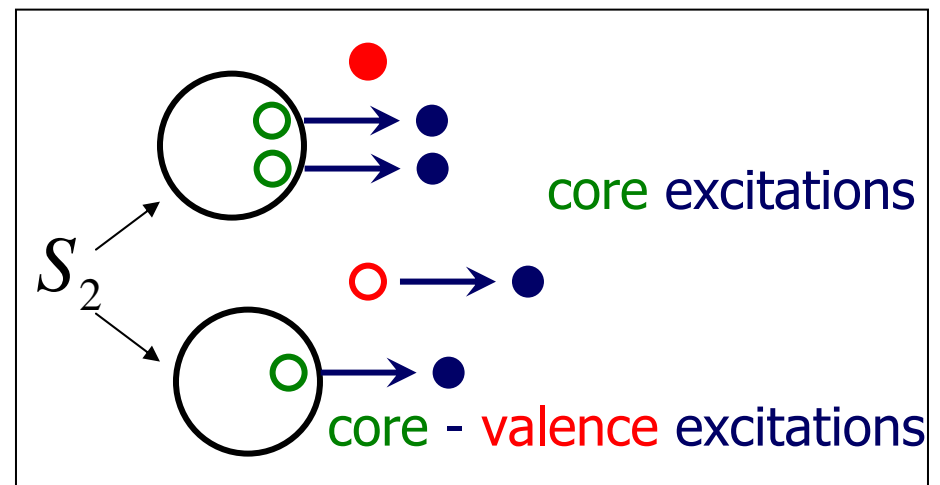
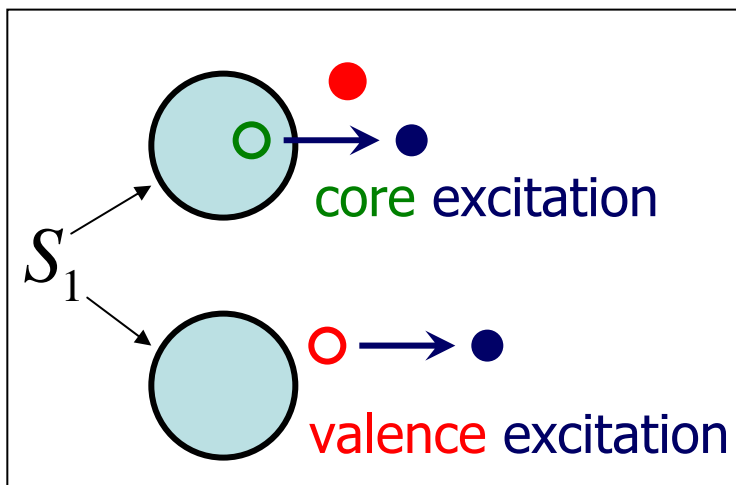
Triple excitations

- Study the effects of this terms
 - Improve accuracy of atomic properties
 - Study fundamental symmetries
 - Better all-order excitation coefficients
- CI + all-order method

COUPLED-CLUSTER METHOD (CCSD)

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

$$\downarrow$$
$$\exp(S_1 + S_2)$$



NON-LINEAR TERMS

$$\exp(S_1 + S_2) = 1 + (S_1 + S_2) + \frac{1}{2!}(S_1 + S_2)^2 + \frac{1}{3!}(S_1 + S_2)^3 + \frac{1}{4!}(S_1 + S_2)^4 + \dots$$

Linear part

Non-linear part

SIX TERMS ONLY !

$$\frac{1}{2}(S_1^2 + 2S_1S_2 + S_2^2) + \frac{1}{6}(S_1^3 + 3S_1^2S_2) + \frac{1}{24}S_1^4$$

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!

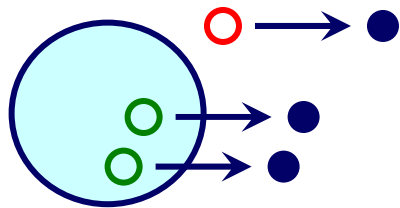
Input: ASCII input of terms of the type

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

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

Triple excitations

- core
- valence electron
- any excited orbital



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

Problem: too many excitation coefficients ρ_{mnrab} .

Triple excitations

Problem: too many excitation coefficients $\rho_{mnr}vab$.

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

The complexity of the equations increases.
Same issue with third-order MBPT for two-particle systems (hundreds of terms) .
What to do with large number of terms?

Solution: automated code generation !

Automated code generation

Codes that write formulas

A diagram illustrating the flow of automated code generation. It consists of two horizontal bars with a blue-to-red gradient. The top bar contains the text 'Codes that write formulas'. A curved arrow points from the right side of this bar down to the right side of the bottom bar, which contains the text 'Codes that write codes'.

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!

EXTENSIONS OF THE ALL ORDER METHOD

Add more terms to the all order wave-function

Non-linear terms  Triple excitations

Non-linear terms:

R. Pal, M.S. Safronova, W.R. Johnson, A. Derevianko, S. G. Porsev, Phys. Rev. A 75, 042515 (2007)

Triple excitations:

S. G. Porsev and A. Derevianko, Phys. Rev. A 73, 012501 (2006) (Na)

A. Derevianko and S. G. Porsev, Eur. Phys. J. A 32 (4), 517(2007) (Cs)

E. Iskrenova-Tchoukova and M.S. Safronova, in progress

SUMMARY OF THEORY METHODS

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

- **Configuration interaction + second-order MBPT**
- Configuration interaction + all-order methods*


*under development

CONFIGURATION INTERACTION METHOD

$$\Psi = \sum_i c_i \Phi_i \leftarrow \begin{array}{l} \text{Single-electron valence} \\ \text{basis states} \end{array}$$
$$(H^{eff} - E)\Psi = 0$$

Example: two particle system:

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

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


CONFIGURATION INTERACTION + MANY-BODY PERTURBATION THEORY

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

MBPT can not accurately describe valence-valence correlation.

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

CONFIGURATION INTERACTION METHOD + MBPT

H_{eff} is modified using perturbation theory expressions

$$\begin{array}{l} h_1 \rightarrow h_1 + \Sigma_1 \\ h_2 \rightarrow h_2 + \Sigma_2 \end{array} \quad \Rightarrow \quad (H^{\text{eff}} - E)\Psi = 0$$

Σ_1, Σ_2 are obtained using perturbation theory

V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov , Phys. Rev. A **54**, 3948 (1996)

V. A. Dzuba and W. R. Johnson , Phys. Rev. A **57**, 2459 (1998)

V. A. Dzuba, V. V. Flambaum, and J. S. Ginges , Phys. Rev. A **61**, 062509 (2000)

S. G. Porsev, M. G. Kozlov, Yu. G. Rakhlina, and A. Derevianko, Phys. Rev. A **64**, 012508 (2001)

M. G. Kozlov, S. G. Porsev, and W. R. Johnson, Phys. Rev. A **64**, 052107 (2001)

I. M. Savukov and W. R. Johnson, Phys. Rev. A **65**, 042503 (2002)

Sergey G. Porsev, Andrei Derevianko, and E. N. Fortson, Phys. Rev. A **69**, 021403 (2004)

V. A. Dzuba and J. S. Ginges, Phys. Rev. A **73**, 032503 (2006)

V. A. Dzuba and V. V. Flambaum , Phys. Rev. A **75**, 052504 (2007)

CONFIGURATION INTERACTION + ALL-ORDER METHOD

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

$$\left(\Sigma_1\right)_{mn} = \left(\epsilon_n - \epsilon_m\right) \rho_{mn}$$

$$\left(\Sigma_2\right)_{mnkl}^L = \left(\epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n\right) \rho_{mnkl}^L$$

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

CI + ALL-ORDER: PRELIMINARY RESULTS

Mg	Experiment		CI	DIF	CI+II	DIF	CI+ALL	DIF
IP		182939	179525	3414	182673	266	182848	91
3s3p ³P	J=0	21850	20899	951	21764	86	21824	26
	J=1	21870	20919	951	21785	85	21843	27
	J=2	21911	20960	951	21829	82	21888	23
3s3p ¹P	J=1	35051	34486	565	35048	3	35061	-10
3s4s ³S	J=1	41197	40392	805	41110	87	41151	46
3s4s ¹S	J=0	43503	42664	839	43428	75	43486	17
3s3d ¹D	J=2	46403	45108	1295	46296	107	46367	36

Ionization potentials

Ca	CI	CI+II	CI+All-order
	-4.1%	0.6%	0.3%
Ba	-6.4%	1.7%	0.5%

M.S. Safronova, M. Kozlov, and W.R. Johnson, in preparation

CONCLUSION

- New evaluation of the spin-dependent PNC amplitude in Cs
- Nuclear anapole moments: need new experiments
- Further development of the all-order method
- Non-linear terms and triple excitations

- Development of CI+ all-order method for PNC studies in more complicated systems: preliminary results demonstrate improvement over the CI+MBPT method



GRADUATE STUDENTS:

BINDIYA ARORA

RUPSI PAL

JENNY TCHOUKOVA

DANSHA JIANG

COLLABORATIONS:

Walter Johnson (University of Notre Dame)

Michael Kozlov (Petersburg Nuclear Physics Institute)

Ulyana Safronova (University of Nevada-Reno)