September 20, 2007

Rare Isotopes & Fundamental symmetries workshop

ATOMIC PNC THEORY: CURRENT STATUS AND FUTURE PROSPECTS

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UNIVERSITY OF DELAWARE

NSF

OUTLINE

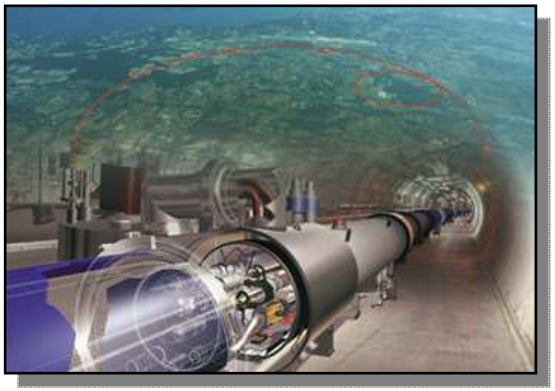
- Motivation & Summary of experiment
- Nuclear spin-independent PNC & weak charge
- How to determine the theoretical uncertainty?
- Nuclear spin-dependent PNC & anapole moments
- Overview of theoretical methods
- All-order method
- CI + all-order method & future prospects

MOTIVATION: PNC I

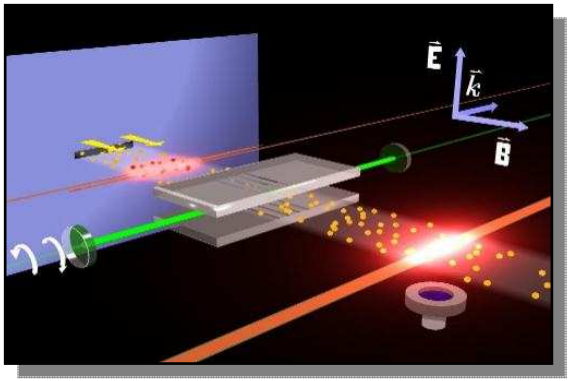
Searches for new physics beyond the Standard Model

High energies

(1) Search for new processes or particles directly



(2) Study (very precisely!) quantities which Standard Model predicts and compare the result with its prediction



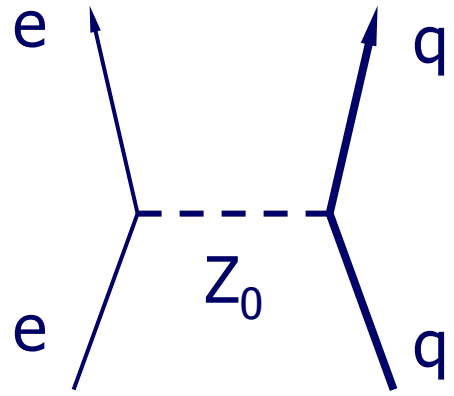
Weak charge Q_W

Low energies

http://public.web.cern.ch/, Cs experiment, University of Colorado

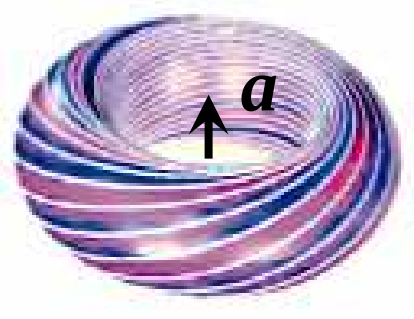
MOTIVATION: PNC

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



Weak Charge Q_W

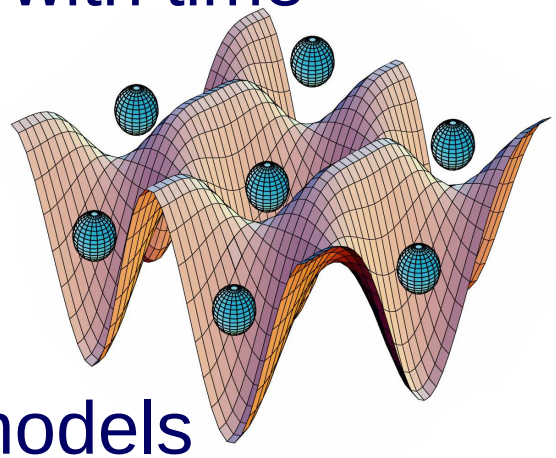
NUCLEAR SPIN-DEPENDENT PNC: STUDY OF PNC IN THE NUCLEUS



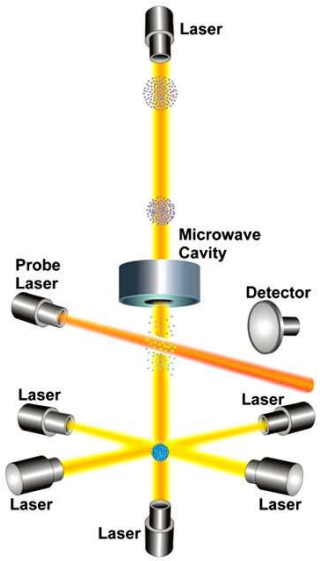
Nuclear anapole moment

MOTIVATION: OTHER

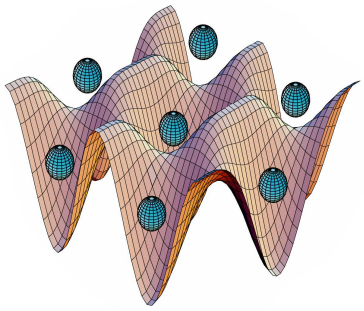
- Benchmark tests of new methodologies
- Search for the EDM
- Variation of fundamental constants with time
- Analysis of various experiments
- Study of long-range interactions
- Other nuclear physics applications
- Astrophysics
- Actinide ion studies for chemistry models
- State-insensitive cooling and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

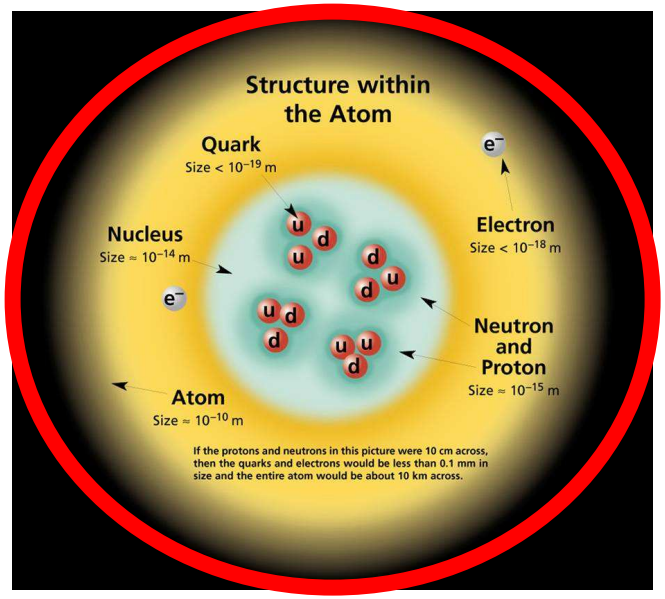


MOTIVATION



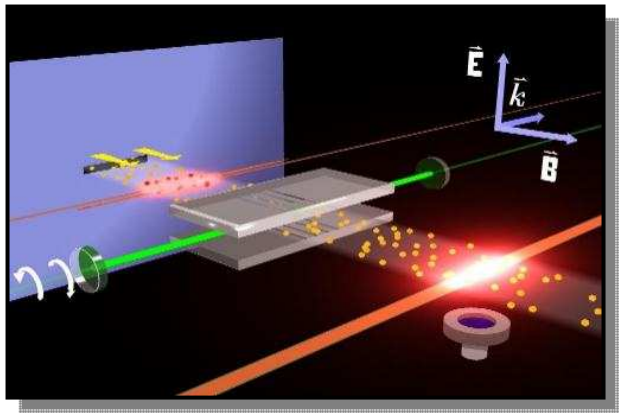
Atomic Clocks

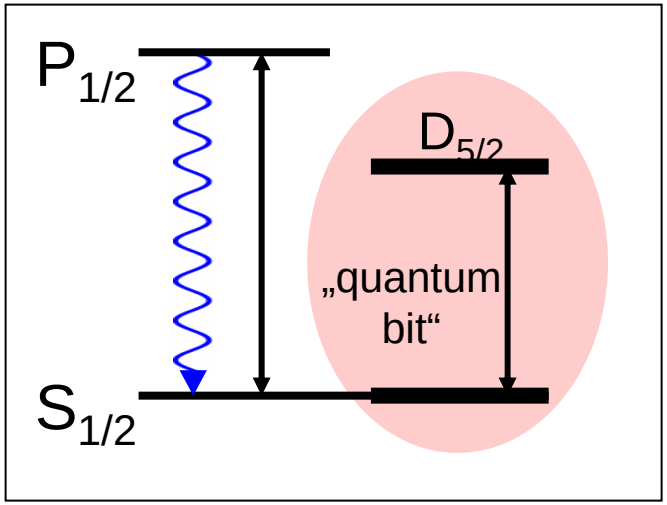




NEED ATOMIC PROPERTIES

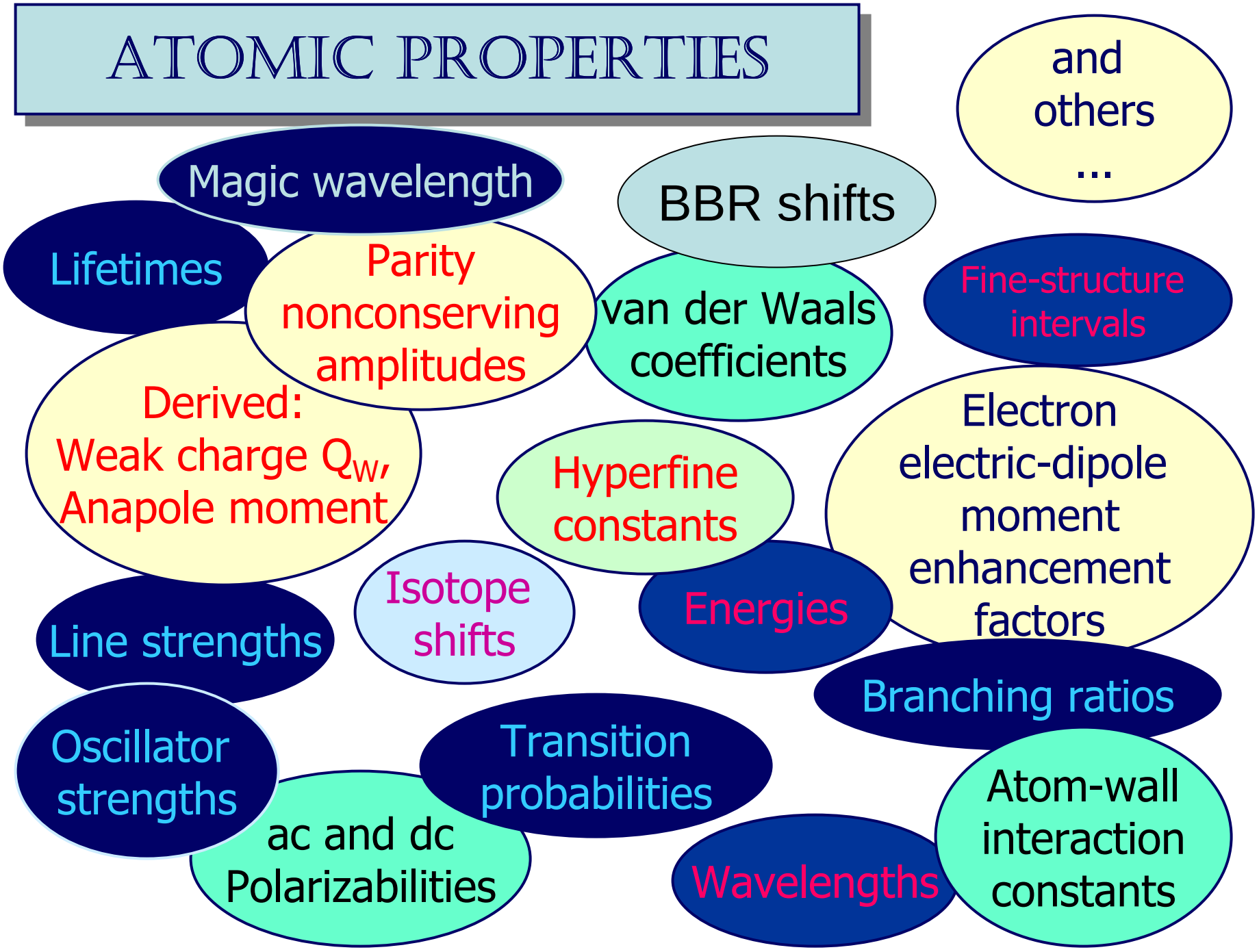
Parity Violation





Quantum information

ATOMIC PROPERTIES

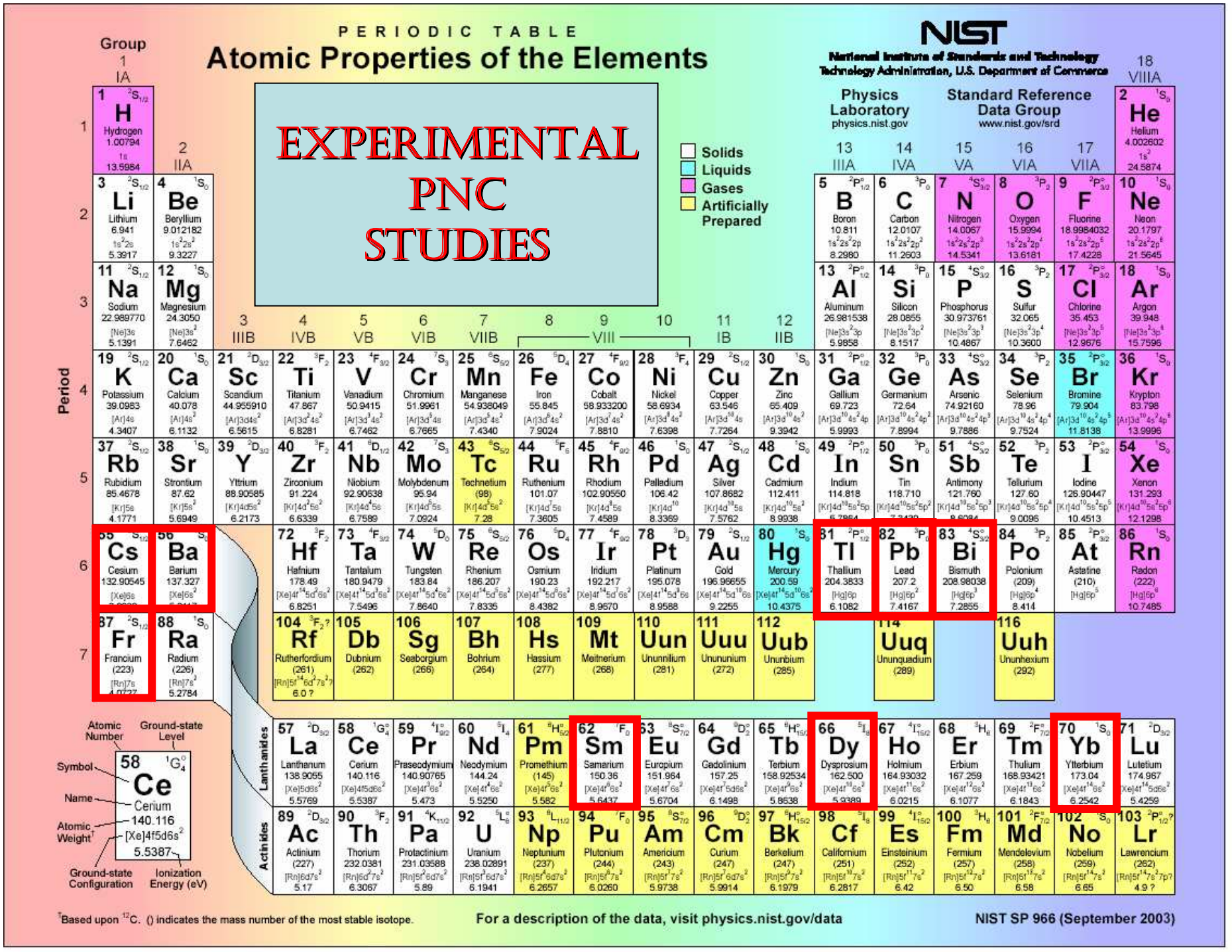


HOW TO ACCURATELY CALCULATE ATOMIC PROPERTIES?

Very precise cal[illegible]n of atomic properties

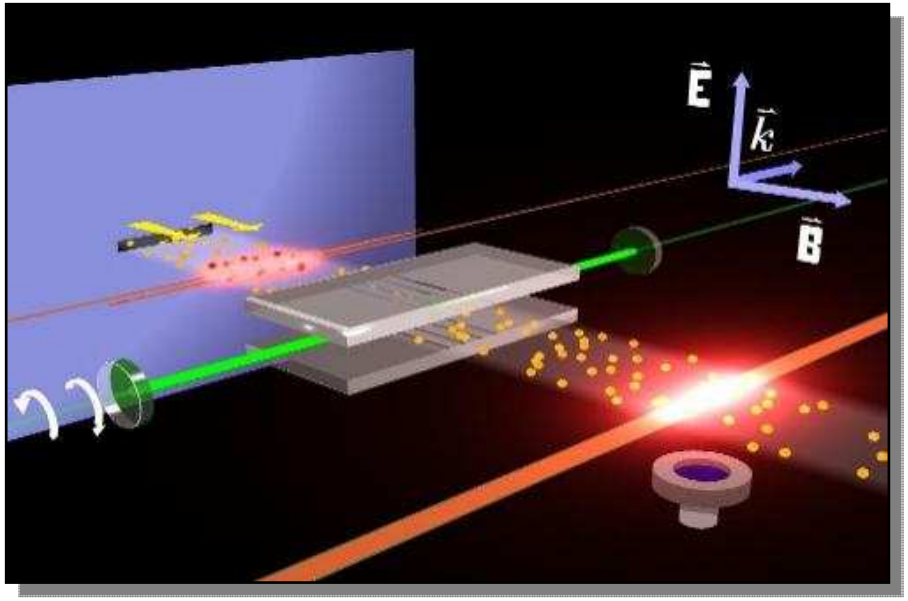
We also need to evaluate uncertainties of theoretical values!

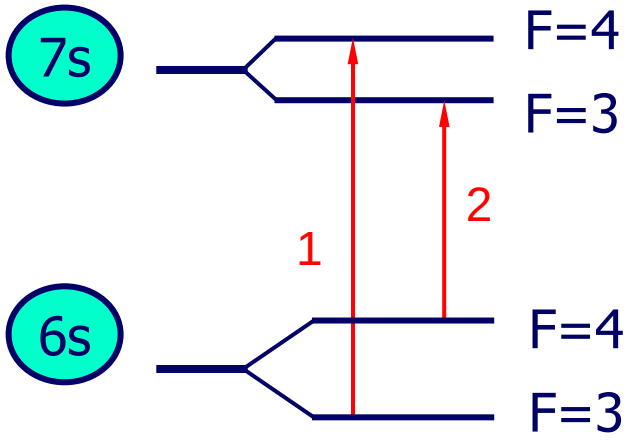
EXPERIMENTAL PNC STUDIES


PERIODIC TABLE
Atomic Properties of the Elements
NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce
Physics Laboratory
physics.nist.gov
Standard Reference Data Group
www.nist.gov/srd
EXPERIMENTAL
PNC
STUDIES
Solids
Liquids
Gases
Artificially Prepared
Group
Period
Lanthanides
Actinides
Atomic Number
Ground-state Level
Symbol
Name
Atomic Weight†
Ground-state Configuration
Ionization Energy (eV)
†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)





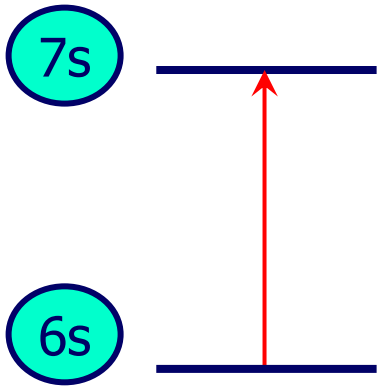
$$\frac{\mathrm{Im}\left(E_{\mathrm{PNC}}\right)}{\beta} = \begin{cases} -1.6349(80)\ {}^{\mathrm{mV}}\!/_{\mathrm{cm}} & 1 \\ -1.5576(77)\ {}^{\mathrm{mV}}\!/_{\mathrm{cm}} & 2 \end{cases}$$

0.3% accuracy

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

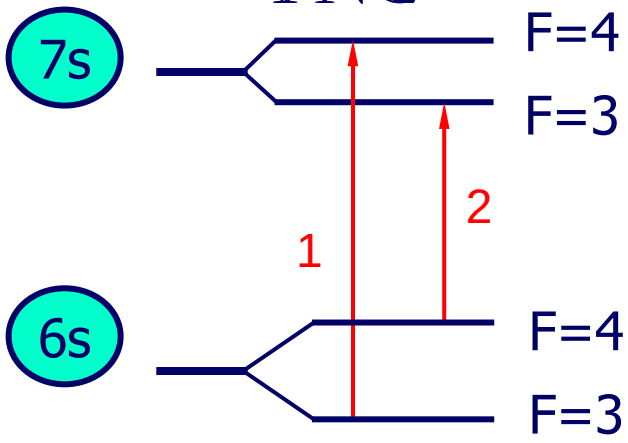


Average of 1 & 2

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

Weak Charge Q_W

NUCLEAR SPIN-DEPENDENT PNC



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

ANALYSIS OF CS PNC EXPERIMENT: THEORY INPUT

Weak Charge Q_W

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

Need theory $E_{\mathrm{PNC}}^{\mathrm{si}}$ calculation in terms of Q_w

Need β

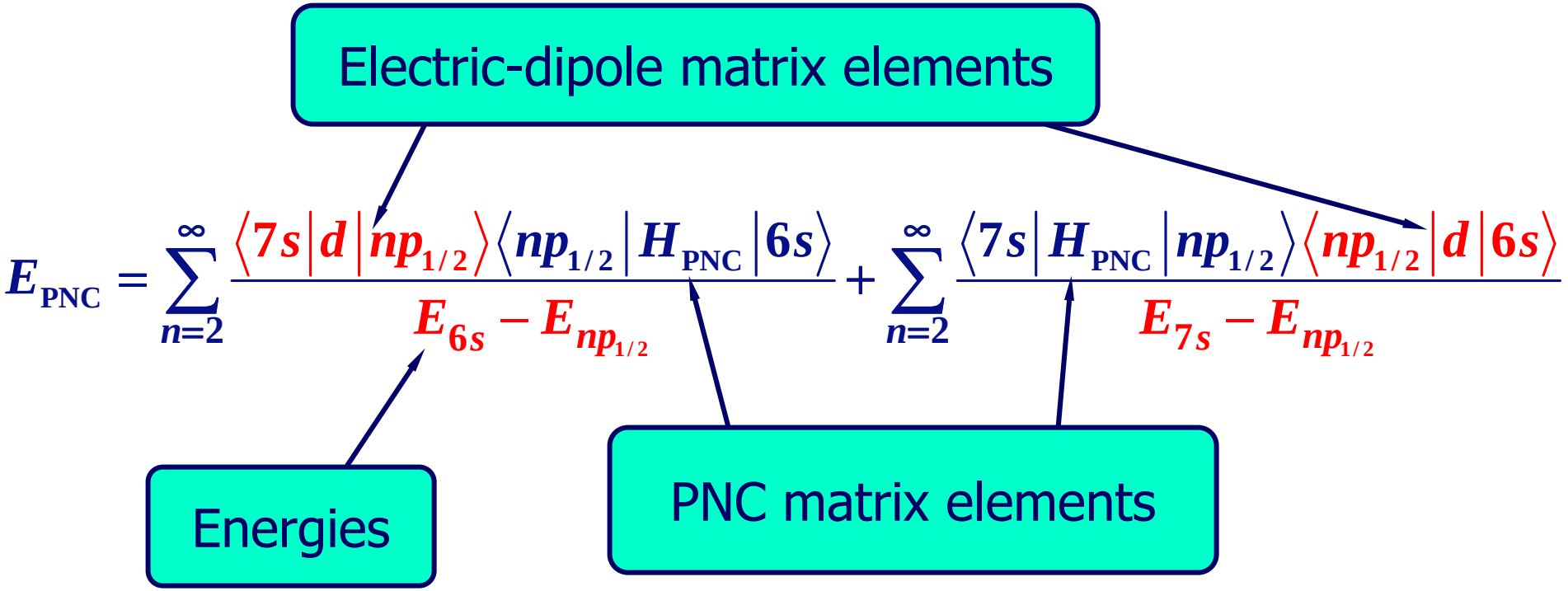
Nuclear anapole moment

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

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

Need β

CALCULATION OF SPIN-INDEPENDENT PNC AMPLITUDE



Nuclear density function

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

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 $M1_{HFS}/\beta$) [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)

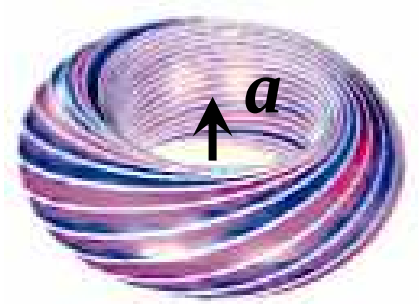
-0.909 Safronova & Johnson (1999)
-0.905 Kozlov et al. (2001)
-0.908 Dzuba et al. (2002) **0.5% uncertainty**

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

DETERMINATION OF Q_W

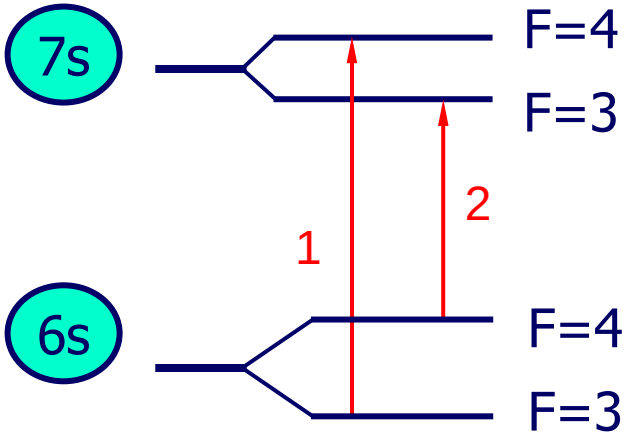
Wood et al. (1997) $\mathrm{Im}(E_{\mathrm{PNC}})/\beta$	-72.11(27)$_{\mathbf{expt}}$(89)$_{\mathbf{theor}}$	1σ
Bennett & Wieman (1999)	-72.06(28)$_{\mathbf{expt}}$(34)$_{\mathbf{theor}}$	2.5σ
Measurement of β		
Derevianko (2000,2002)	-72.61(28)$_{\mathbf{expt}}$(34/73)$_{\mathbf{theor}}$	1.3σ/0.7σ
Calculation of Breit correction		
Dzuba et al. (2000)	-72.42(28)$_{\mathbf{expt}}$(74)$_{\mathbf{theor}}$	1.5σ/no dev.
Calculation of Breit correction		
Kozlov et al. (2001)	-72.5(7)	no deviation
Calculation of E_{PNC}, Breit correction		
Johnson et al. (2001)	-72.12(28)$_{\mathbf{expt}}$(34/74)$_{\mathbf{theor}}$	2.2σ/1.2σ
Calculation of vacuum pol. corr.		
Milstein & Sushkov (2002)		2.2σ
Calculation of vacuum pol. corr.		
Vasilyev et al. (2002)	-72.65(49)	1.1σ
Measurement of 6s-7p trans., β		
Dzuba et al. (2002) E_{PNC}	-72.16(29)$_{expt}$(36)$_{th}$	2σ
Flambaum & Kuchiev (2002)	-72.71(29)$_{expt}$(36)$_{th}$	no deviation
Milstein et al. (2003)		
self-energy & vertex corr.	-72.81(28)$_{expt}$(36)$_{th}$	0.6σ

SPIN-DEPENDENT PARITY VIOLATION: NUCLEAR ANAPOLE MOMENT



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

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

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

+

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

+

Experimental or theoretical value of vector transition polarizability β

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

$\kappa \neq \kappa_a$ More spin-dependent PNC effects!

W.R. Johnson, M.S. Safronova and U.I. Safronova, Phys. Rev. A 67, 062106 (2003)

MORE SPIN-DEPENDENT PNC EFFECTS

$$\kappa = \kappa_a + \kappa_2 + \kappa_{\mathrm{hf}}$$

(V_e, A_N) interaction

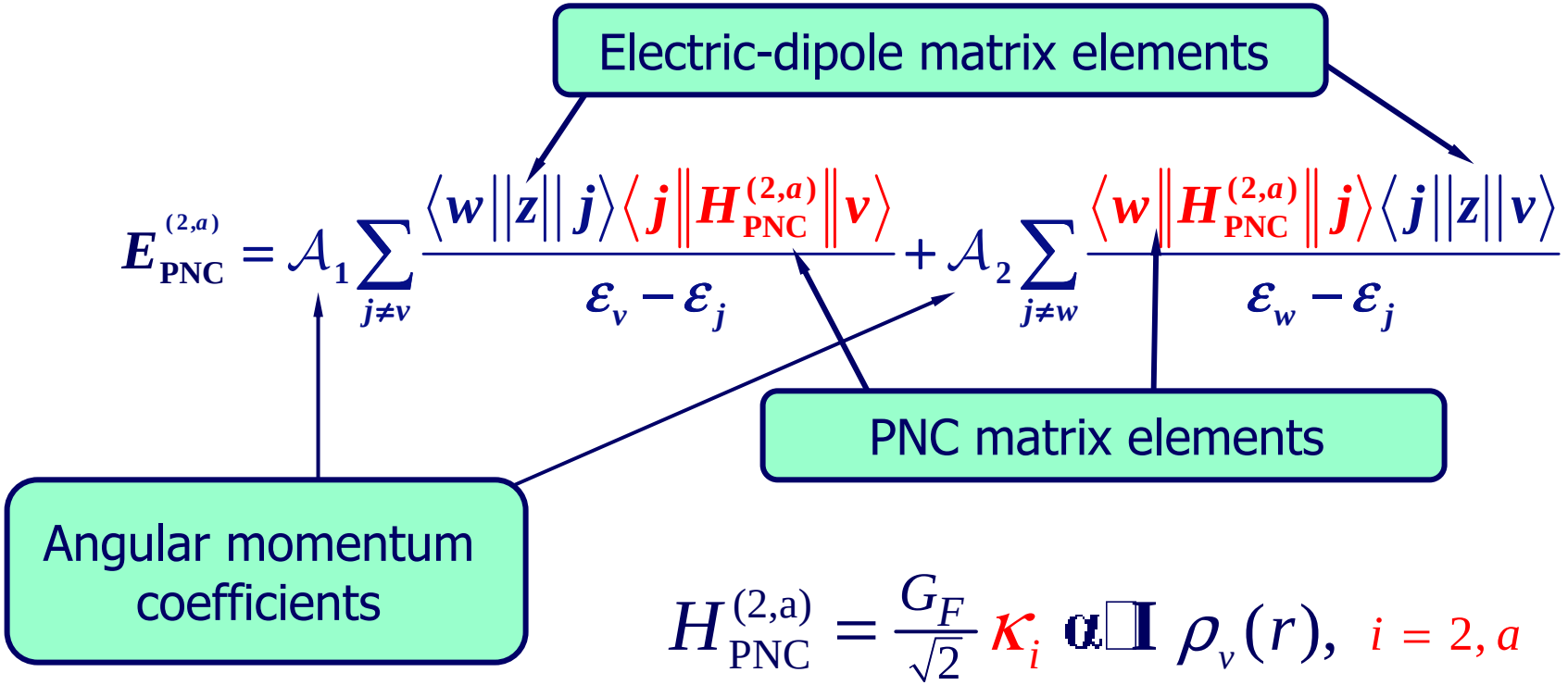
Weak-hyperfine interference term

Same Hamiltonian as anapole moment term with $\kappa_a \Rightarrow \kappa_2$

This term does not reduce to the same interaction but "effective" constant κ_{hf} can be calculated.

W.R. Johnson, M.S. Safronova and U.I. Safronova, Phys. Rev. A 67, 062106 (2003)

ANAPOLE MOMENT AND AXIAL-VECTOR TERMS



$$H_{\mathrm{PNC}}^{(2,\mathrm{a})} = \frac{G_F}{\sqrt{2}} \kappa_i \, \alpha \, \rho_v(r), \quad i = 2, a$$

WEAK-HYPERFINE INTERFERENCE TERM κ_{hf}

Hyperfine

Spin-independent PNC

E1

$$\langle wIF_FM_F|z|vIF_IM_I\rangle^{(\mathrm{hf})} =$$

$$\sum_{\substack{m\neq w\\ n\neq w}} \frac{\langle w|H^{(1)}|n\rangle\langle n|H^{(\mathrm{hf})}|m\rangle\langle m|z|v\rangle}{(E_w-E_m)(E_w-E_n)} + \sum_{\substack{m\neq w\\ n\neq w}} \frac{\langle w|H^{(\mathrm{hf})}|n\rangle\langle n|H^{(1)}|m\rangle\langle m|z|v\rangle}{(E_w-E_m)(E_w-E_n)}$$

$$+ \sum_{\substack{m\neq w\\ n\neq v}} \frac{\langle w|H^{(1)}|m\rangle\langle m|z|n\rangle\langle n|H^{(\mathrm{hf})}|v\rangle}{(E_w-E_m)(E_v-E_n)} + \sum_{\substack{m\neq w\\ n\neq v}} \frac{\langle w|H^{(\mathrm{hf})}|m\rangle\langle m|z|n\rangle\langle n|H^{(1)}|v\rangle}{(E_w-E_m)(E_v-E_n)}$$

$$+ \sum_{\substack{m\neq v\\ n\neq v}} \frac{\langle w|z|n\rangle\langle n|H^{(1)}|m\rangle\langle m|H^{(\mathrm{hf})}|v\rangle}{(E_v-E_m)(E_v-E_n)} + \sum_{\substack{m\neq v\\ n\neq v}} \frac{\langle w|z|n\rangle\langle n|H^{(\mathrm{hf})}|m\rangle\langle m|H^{(1)}|v\rangle}{(E_v-E_m)(E_v-E_n)}$$

$$-\langle w|H^{(\mathrm{hf})}|w\rangle \sum_{m\neq w} \frac{\langle w|H^{(1)}|m\rangle\langle m|z|v\rangle}{(E_w-E_m)^2} - \sum_{n\neq v} \frac{\langle w|z|n\rangle\langle n|H^{(1)}|v\rangle}{(E_v-E_n)^2}\langle v|H^{(\mathrm{hf})}|v\rangle,$$

NUCLEAR ANAPOLE MOMENT: SUMMARY

Group	κ	κ_2	$\kappa_{\rm hf}$	κ_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	

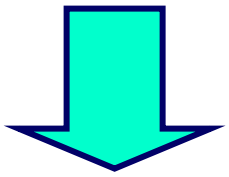
[1] W.R. Johnson, M.S. Safronova and U.I. Safronova, Phys. Rev. A 67, 062106 (2003)
[2] W. C. Haxton, C.-P. Liu, and M. J. Ramsey-Musolf, Phys. Rev. Lett. 86, 5247 (2001)
[3] V. V. Flambaum and D. W. Murray, Phys. Rev. C 56, 1641 (1997)
[4] C. Bouchiat and C. A. Piketty, Phys. Lett. B 269, 195 (1991)

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.

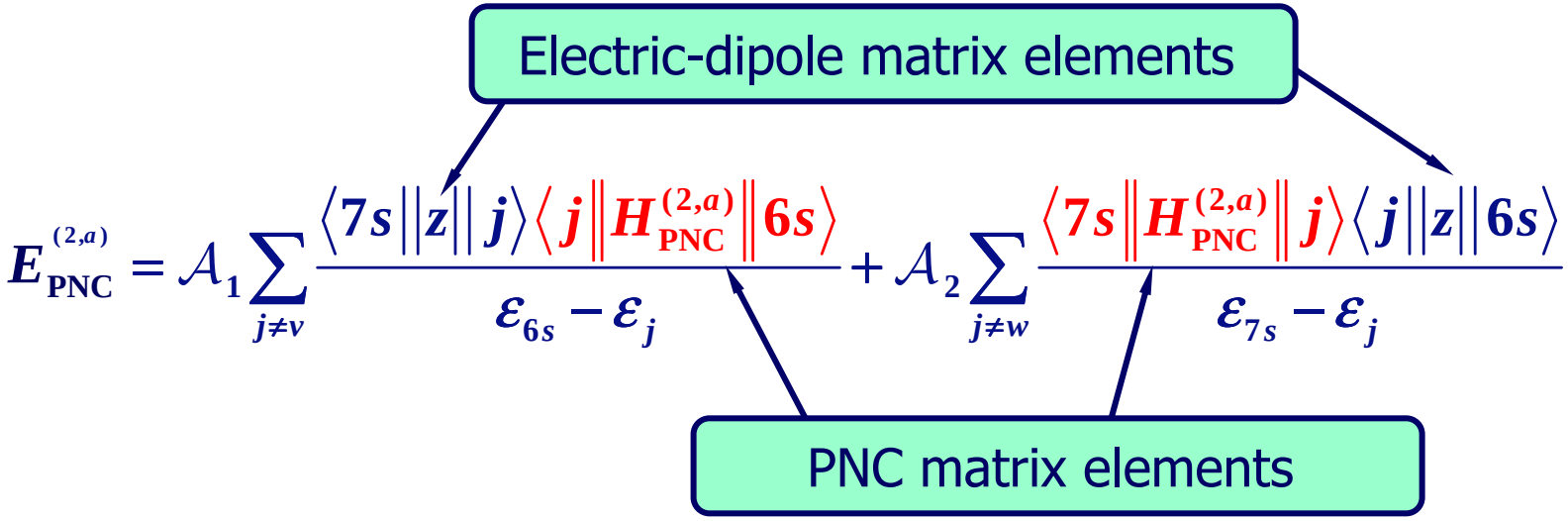
Possible atomic calculation solution?

$\kappa = 0.117(16)$



Incomplete correlation calculation of spin-dependent PNC amplitude?

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



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:

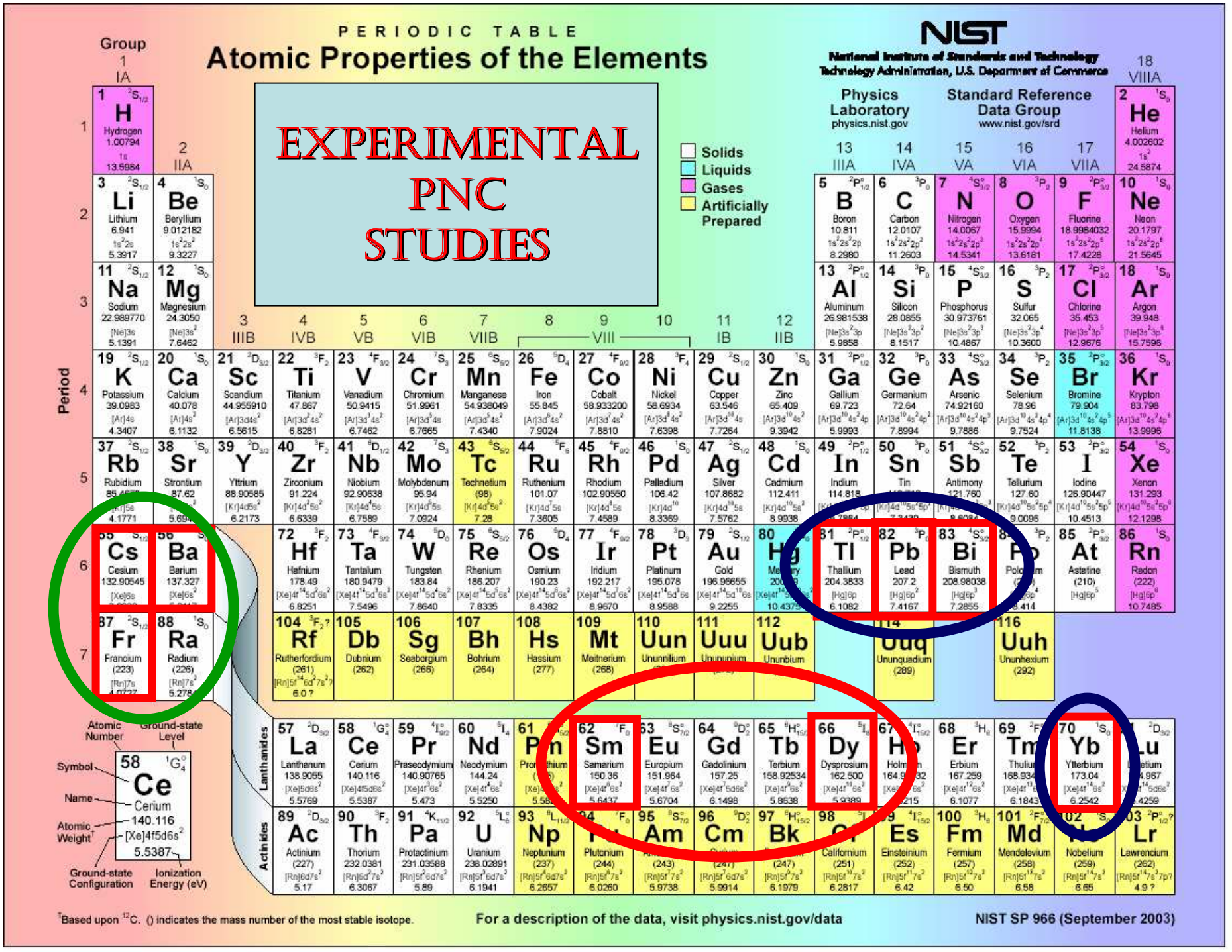
$\kappa = 0.110(16)$*

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?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PNC
STUDIES
Solids
Liquids
Gases
Artificially Prepared
Group
Period
Lanthanides
Actinides
Atomic Number
Ground-state Level
Symbol
Name
Atomic Weight†
Ground-state Configuration
Ionization Energy (eV)
†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

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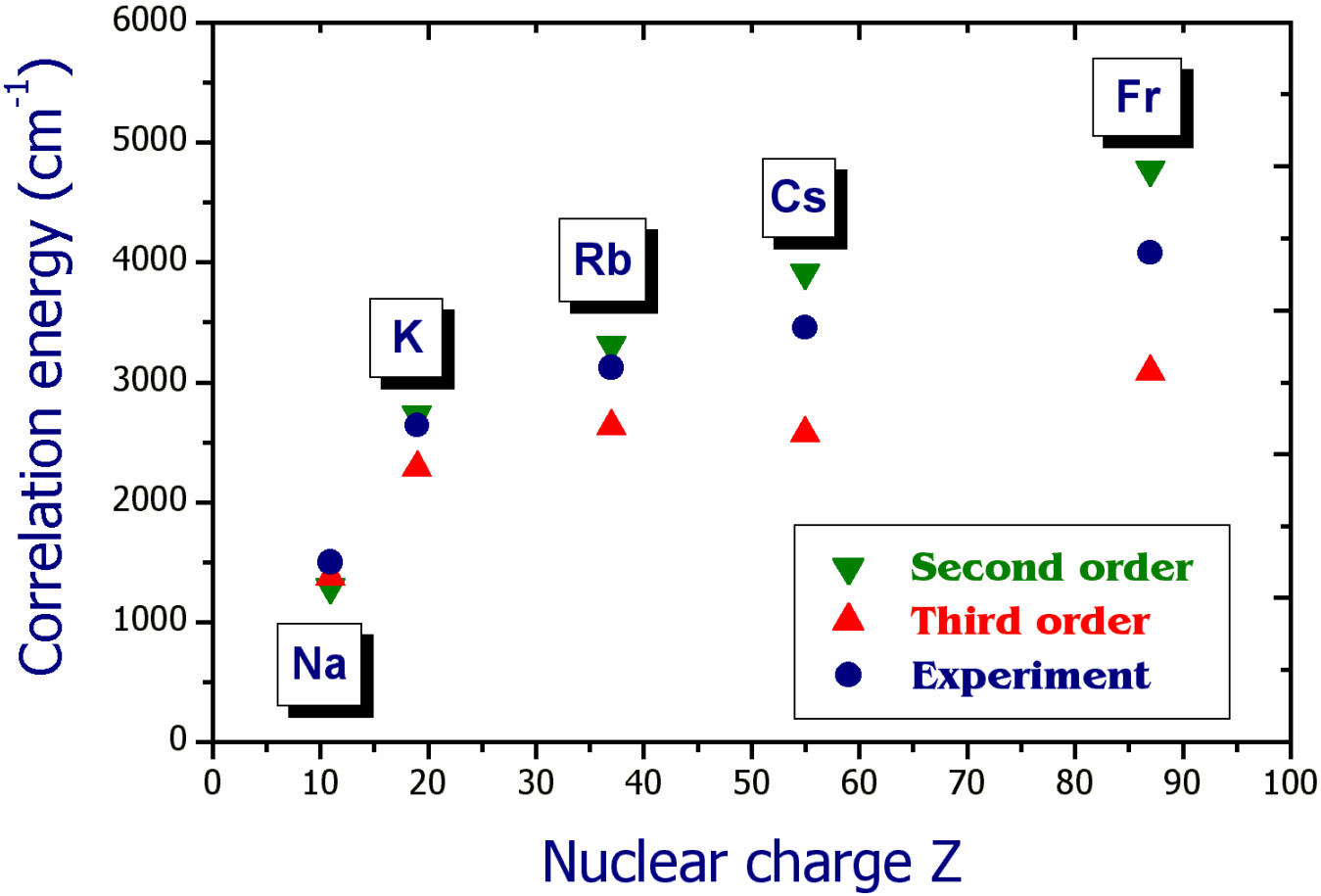
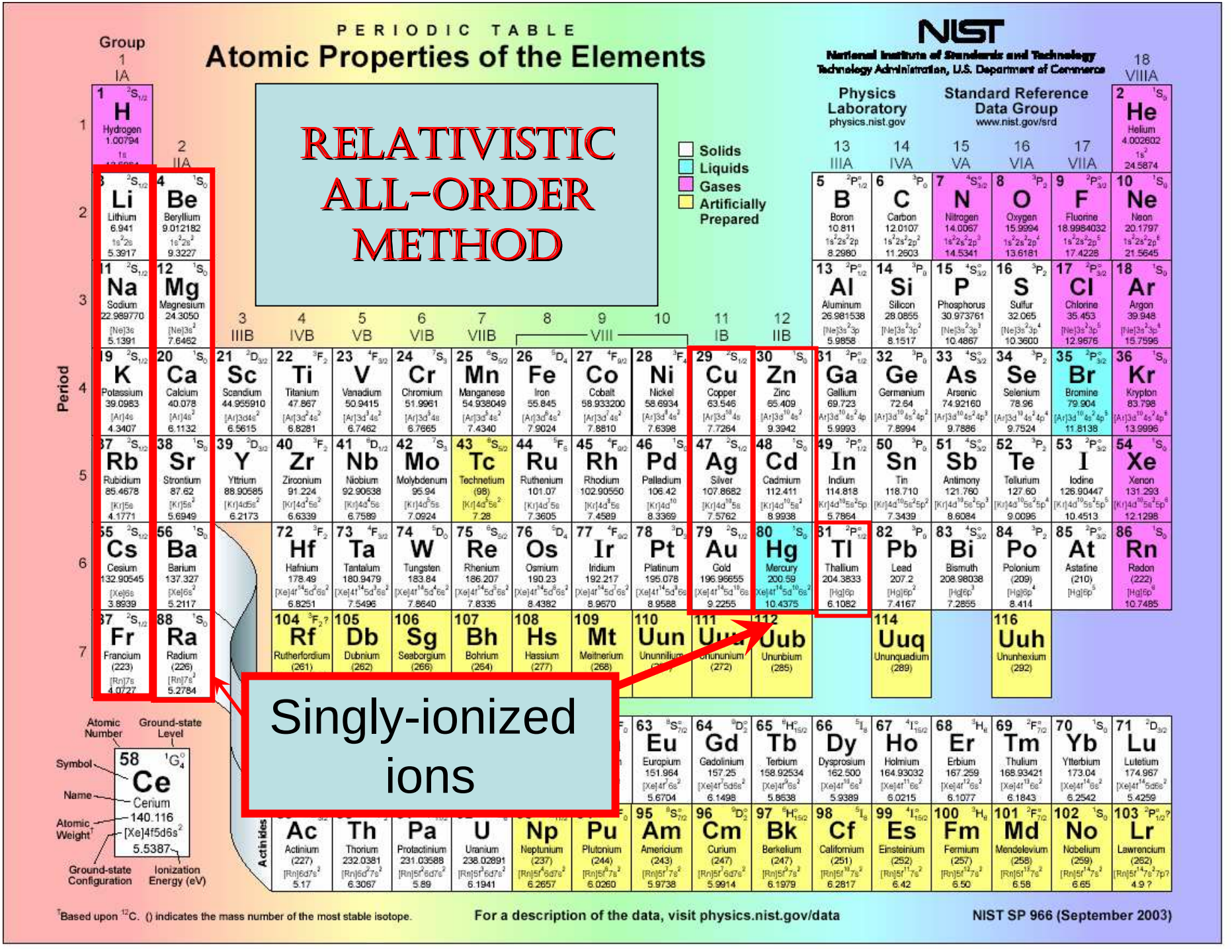
*under development

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
Physics Laboratory
physics.nist.gov
Standard Reference Data Group
www.nist.gov/srd
RELATIVISTIC ALL-ORDER METHOD
Solids
Liquids
Gases
Artificially Prepared
Singly-ionized ions
Group
Period
Actinides
Atomic Number
Ground-state Level
Symbol
Name
Atomic Weight†
Ground-state Configuration
Ionization Energy (eV)
†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)

RELATIVISTIC ALL-ORDER METHOD

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

Scheme:

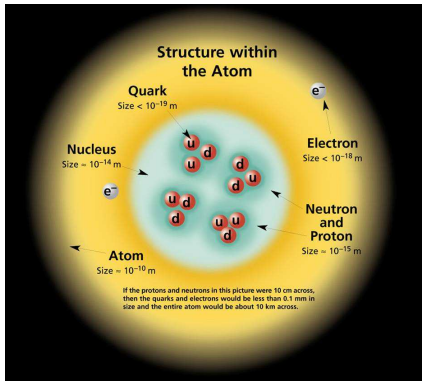
Calculate the atomic wave functions and energies

↓

Calculate various matrix elements

↓

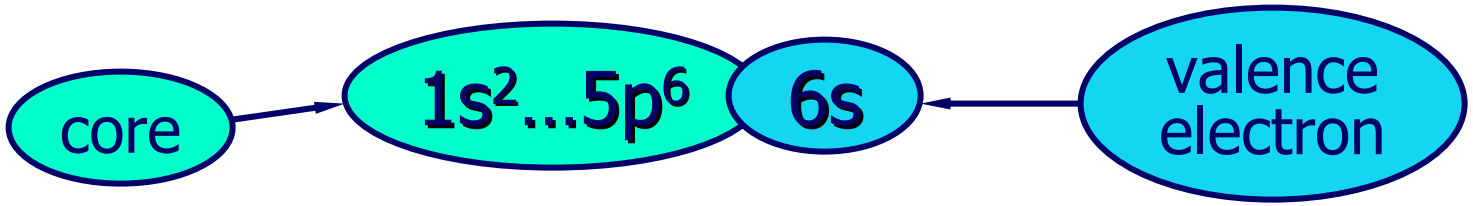
Calculate "derived" properties such as PNC amplitudes



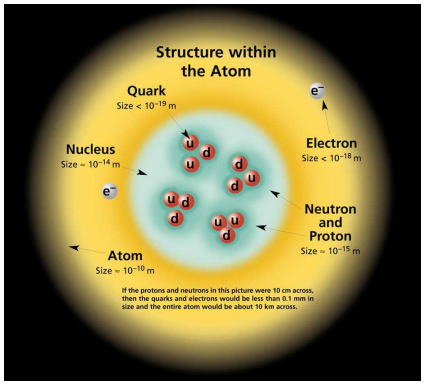
LOWEST ORDER

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.

core — $1s^2 \ldots 5p^6$ — 6s — valence electron

Lowest-order wave function

$$\left|\Psi_v^{(0)}\right\rangle = a_v^\dagger \left|\Psi_{core}\right\rangle$$

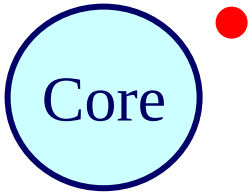
Core

Creation operator for state v

Core wave function

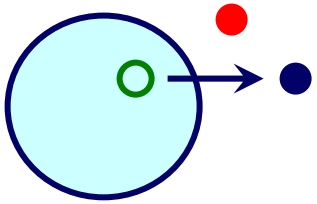
ALL-ORDER ATOMIC WAVE FUNCTION (SD)

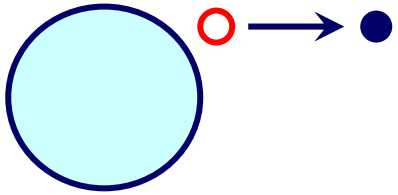
Lowest order



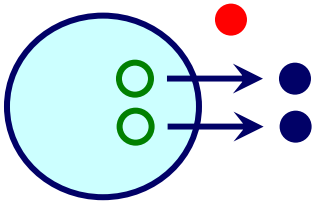
core
valence electron
any excited orbital

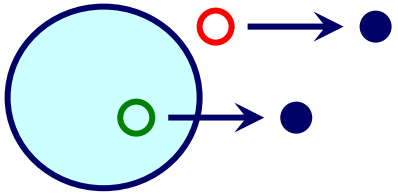
Single-particle excitations





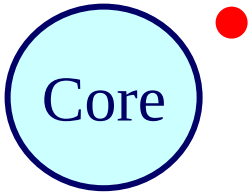
Double-particle excitations





ALL-ORDER ATOMIC WAVE FUNCTION (SD)

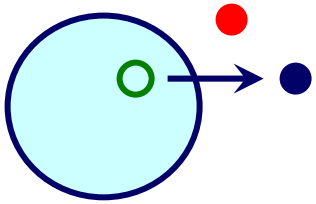
Lowest order



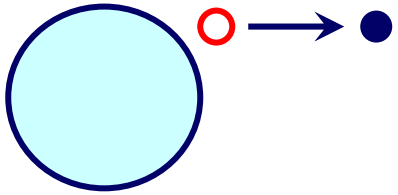
$$\left|\Psi_v^{(0)}\right\rangle$$

- core
- valence electron
- any excited orbital

Single-particle excitations

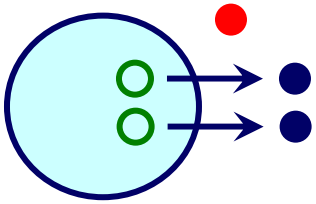


$$\sum_{ma} \rho_{ma}\, a_m^\dagger a_a \left|\Psi_v^{(0)}\right\rangle$$

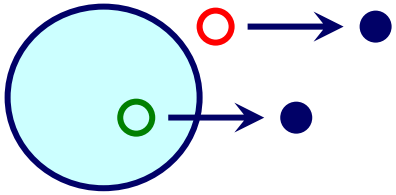


$$\sum_{m\neq v} \rho_{mv}\, a_m^\dagger a_v \left|\Psi_v^{(0)}\right\rangle$$

Double-particle excitations



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



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

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 : *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: $\sum_{rs} g_{mnrs}\rho_{rsab}$

a,b core (17 shells)

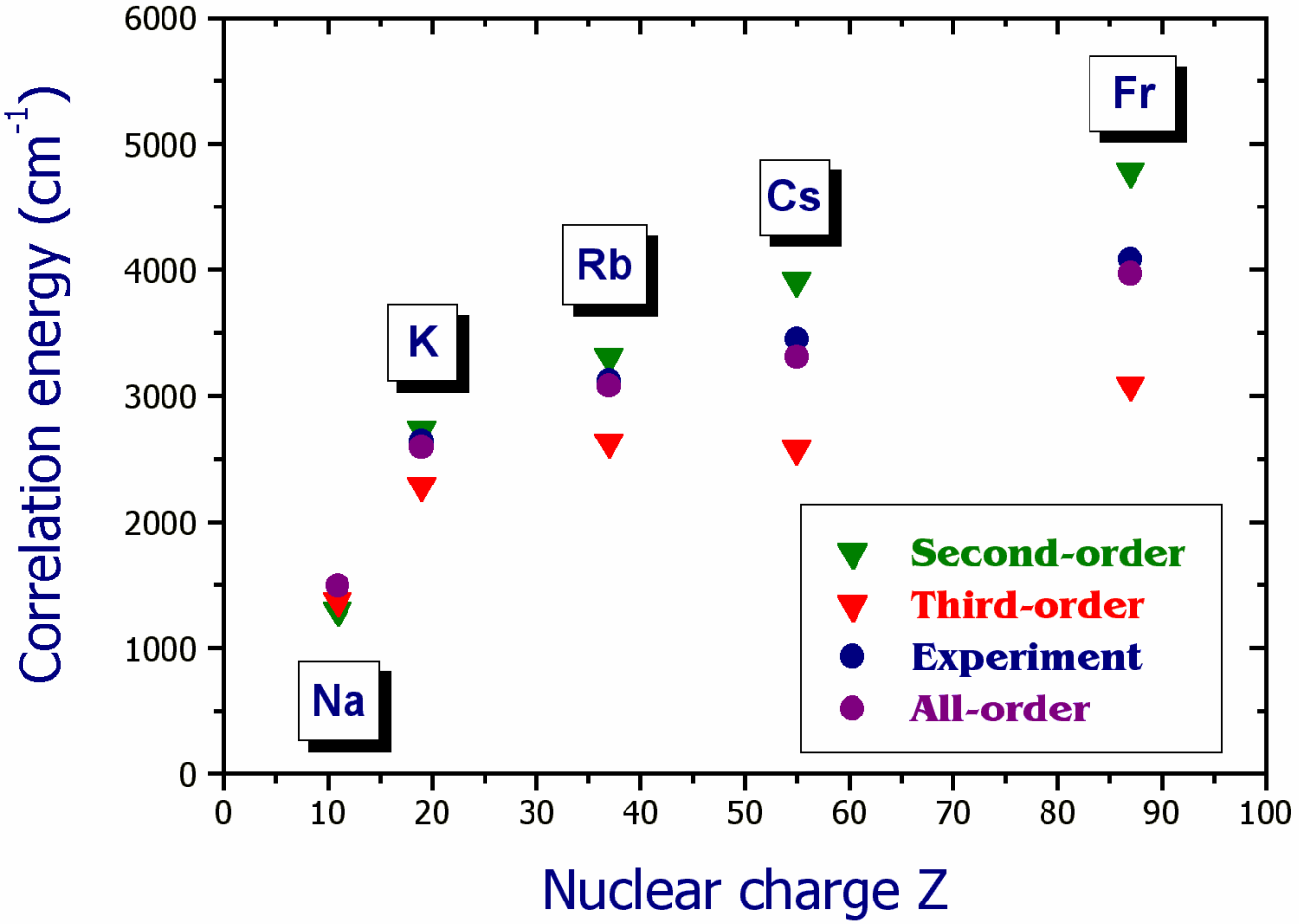
Indices *mnrs* can be ANY orbitals

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

$17x17x(35x13)^4=5 \times 10^{12}$!

- 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?

$$Z_{wv}^{PNC} = \frac{\langle \Psi_w | H_{PNC} | \Psi_v \rangle}{\sqrt{\langle \Psi_w | \Psi_w \rangle \langle \Psi_v | \Psi_v \rangle}} \rightarrow z_{wv}^{(0)} + z^{(a)} + \ldots + z^{(t)}$$

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

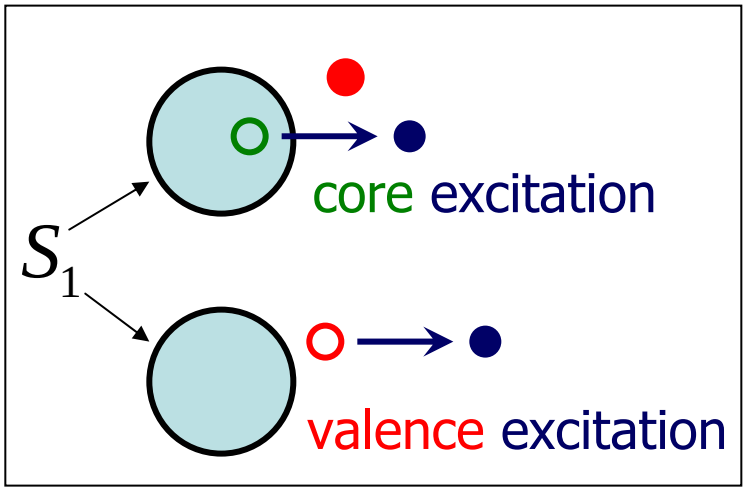
- Study the effects of this terms
- Improve accuracy of atomic properties
- Study fundamental symmetries
- Better all-order excitation coefficients
  CI + all-order method

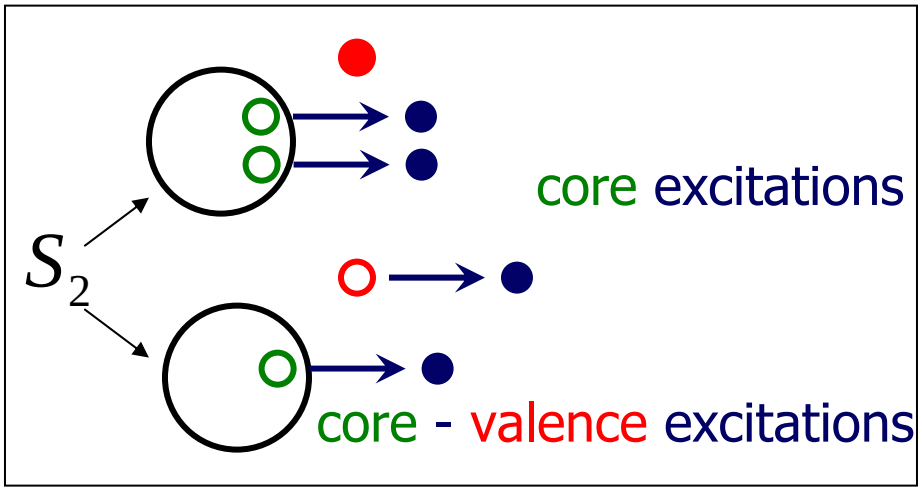
COUPLED-CLUSTER METHOD (CCSD)

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

$$\Downarrow$$

$$\exp(S_1 + S_2)$$





NON-LINEAR TERMS

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

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

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

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!

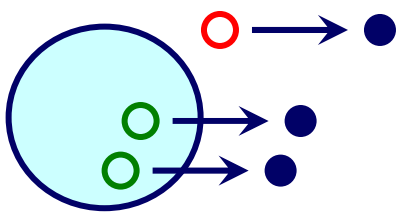
Input: ASCII input of terms of the type

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

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

Triple excitations

- core
- valence electron
- any excited orbital



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

Problem: too many excitation coefficients ρ_{mnrvab}.

Triple excitations

Problem: too many excitation coefficients ρ_{mnrvab} .

Doubles:

ρ_{mnab}

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

m,n : *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!

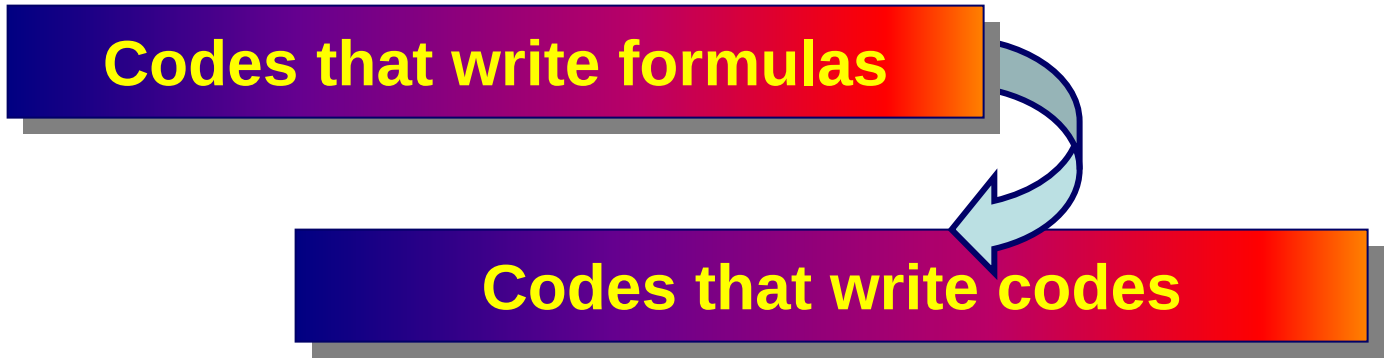
The complexity of the equations also increases.

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

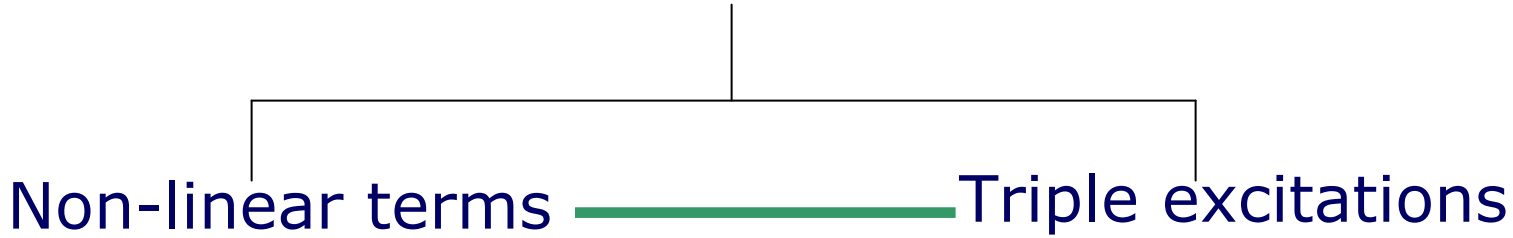


Input: list of formulas to be programmed
Output: final code (need to be put into a main shell)

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:
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

$$\Psi = \sum_i c_i \Phi_i \leftarrow$$ Single-electron valence basis states

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

Example: two particle system:

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

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

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

$$h_1 \to h_1 + \Sigma_1$$
$$h_2 \to h_2 + \Sigma_2$$

$$\Rightarrow \left(H^{eff} - E\right)\Psi = 0$$

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

$$\left(\Sigma_1\right)_{mn} = \left(\varepsilon_n - \varepsilon_m\right)\rho_{mn}$$

$$\left(\Sigma_2\right)^L_{mnkl} = \left(\varepsilon_k + \varepsilon_l - \varepsilon_m - \varepsilon_n\right)\rho^L_{mnkl}$$

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 ^{3}P	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 ^{1}P	J=1	35051	34486	565	35048	3	35061	-10
3s4s ^{3}S	J=1	41197	40392	805	41110	87	41151	46
3s4s ^{1}S	J=0	43503	42664	839	43428	75	43486	17
3s3d ^{1}D	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

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