ATOMIC PNC THEORY: CURRENT STATUS AND FUTURE PROSPECTS

MARIANNA SAFRONOVA
• 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
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

Weak charge $Q_W$

High energies

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

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

Weak Charge $Q_W$

Nuclear anapole moment
• 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

P$_{1/2}$

D$_{5/2}$

S$_{1/2}$

"quantum bit"
ATOMIC PROPERTIES

Lifetimes

Parity nonconserving amplitudes

Derived:
Weak charge $Q_w$, Anapole moment

Line strengths

Oscillator strengths

Isotope shifts

ac and dc Polarizabilities

Transition probabilities

Energies

Wavelengths

Branching ratios

Electron electric-dipole moment enhancement factors

Hyperfine constants

van der Waals coefficients

BBR shifts

Fine-structure intervals

Atom-wall interaction constants

Electron

Magic wavelength

Oscillator strengths

Transition probabilities

Ac and dc Polarizabilities

Derived:
Weak charge $Q_w$, Anapole moment

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Van der Waals coefficients

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Lifetimes

Energy

Wavelengths

Branching ratios

Derived:
Weak charge $Q_w$, Anapole moment

Parity nonconserving amplitudes

ATOMIC PROPERTIES

and others...

...
How to accurately calculate atomic properties?

Very precise calculation of atomic properties is wanted!

We also need to evaluate uncertainties of theoretical values!
EXPERIMENTAL PNC STUDIES
Stark interference scheme to measure ratio of the PNC amplitude and the Stark-induced amplitude $\beta$

\[
\frac{\text{Im}(E_{\text{PNC}})}{\beta} = \begin{cases} 
-1.6349(80) \text{ mV/cm} & \text{1} \\
-1.5576(77) \text{ mV/cm} & \text{2}
\end{cases}
\]
**ANALYSIS OF CS PNC EXPERIMENT**

**NUCLEAR SPIN-INDEPENDENT PNC**

- $7s$
- $6s$

Average of 1 & 2

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

**Weak Charge $Q_W$**

**NUCLEAR SPIN-DEPENDENT PNC**

- $7s$
- $6s$

Difference of 1 & 2

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

**Nuclear anapole moment**
ANALYSIS OF CS PNC EXPERIMENT: THEORY INPUT

Weak Charge $Q_w$

\[
\text{Im} \left( \frac{E^{si}_{PNC}}{\beta} \right) = -1.5935(56) \text{ mV/cm}
\]

Need theory calculation in terms of $Q_w$

Need $\beta$

Nuclear anapole moment

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

Need theory calculation in terms of anapole moment

Need $\beta$
CALCULATION OF SPIN-INDEPENDENT PNC AMPLITUDE

Electric-dipole matrix elements

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

Energies

PNC matrix elements

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

Nuclear density function

\[ G_F \text{- Universal Fermi coupling constant} \]
\[ \gamma_5 \text{- Dirac matrix} \]
Tensor transition polarizability $\beta$ 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 $M_{1HFS}/\beta$) [3]: $27.02(8)a_0^3$

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

<table>
<thead>
<tr>
<th>Energies</th>
<th>Dipole</th>
<th>PNC</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>DHF</td>
<td>DHF</td>
<td>DHF</td>
<td>0.735</td>
</tr>
<tr>
<td>Expt.</td>
<td>SD</td>
<td>SD</td>
<td>0.894</td>
</tr>
<tr>
<td>Expt.</td>
<td>“best values”</td>
<td>SD</td>
<td>0.892</td>
</tr>
<tr>
<td>Expt.</td>
<td>SD scaled</td>
<td>SD scaled</td>
<td>0.899</td>
</tr>
<tr>
<td>Expt.</td>
<td>“best values”</td>
<td>SD scaled</td>
<td>0.882</td>
</tr>
</tbody>
</table>

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.
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
<table>
<thead>
<tr>
<th>Study</th>
<th>Lifetime</th>
<th>Experimental</th>
<th>Theoretical</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dzuba et al. (2000,2002)</td>
<td></td>
<td>-72.61(28)</td>
<td>-72.42(28)</td>
<td>1.3σ/0.7σ</td>
</tr>
<tr>
<td>Kozlov et al. (2001)</td>
<td></td>
<td>-72.5(7)</td>
<td></td>
<td>no deviation</td>
</tr>
<tr>
<td>Johnson et al. (2001)</td>
<td></td>
<td>-72.12(28)</td>
<td>-72.16(29)</td>
<td>2.2σ/1.2σ</td>
</tr>
<tr>
<td>Milstein &amp; Sushkov (2002)</td>
<td></td>
<td></td>
<td>-72.65(49)</td>
<td>1.1σ</td>
</tr>
<tr>
<td>Vasilyev et al. (2002)</td>
<td></td>
<td></td>
<td>-72.16(29)</td>
<td>2σ</td>
</tr>
<tr>
<td>Milstein et al. (2003)</td>
<td></td>
<td></td>
<td>-72.81(28)</td>
<td>0.6σ</td>
</tr>
</tbody>
</table>
Parity-violating nuclear moment

\[ H^{(a)}_{\text{PNC}} = \frac{G_F}{\sqrt{2}} \kappa_a \alpha \cdot I \rho_v(r) \]

Anapole moment

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

Valence nucleon density

**SPIN-DEPENDENT PARITY VIOLATION: NUCLEAR ANAPOLE MOMENT**
Experimental value

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

Theoretical value of spin-dependent PNC amplitude in terms of \( \kappa_a \)

Experimental or theoretical value of vector transition polarizability \( \beta \)

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

\( \kappa \neq \kappa_a \) More spin-dependent PNC effects!

Weak-hyperfine interference term $(V_e, A_N)$ interaction

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

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

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

$E_{\text{PNC}}^{(2,a)} = A_1 \sum_{j \neq v} \langle w | z | j \rangle \langle j | H^{(2,a)}_{\text{PNC}} | v \rangle \left( \varepsilon_v - \varepsilon_j \right) + A_2 \sum_{j \neq w} \langle w | H^{(2,a)}_{\text{PNC}} | j \rangle \langle j | z | v \rangle \left( \varepsilon_w - \varepsilon_j \right)$

Angular momentum coefficients

Electric-dipole matrix elements

PNC matrix elements

$H^{(2,a)}_{\text{PNC}} = \frac{G_F}{\sqrt{2}} K_i \alpha \mathbf{I} \rho_v(r), \quad i = 2, a$
\[
\langle w | I F F M | z | v I F I M \rangle^{(hf)} = \sum_{m \neq w} \sum_{n \neq w} \frac{\langle w | H^{(1)} | n \rangle \langle n | H^{(hf)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)(E_w - E_n)} + \sum_{m \neq w} \sum_{n \neq w} \frac{\langle w | H^{(hf)} | n \rangle \langle n | H^{(1)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)(E_w - E_n)} \\
+ \sum_{m \neq w} \sum_{n \neq w} \frac{\langle w | H^{(1)} | m \rangle \langle m | z | n \rangle \langle n | H^{(hf)} | v \rangle}{(E_w - E_m)(E_v - E_n)} + \sum_{m \neq w} \sum_{n \neq w} \frac{\langle w | H^{(hf)} | m \rangle \langle m | z | n \rangle \langle n | H^{(1)} | v \rangle}{(E_w - E_m)(E_v - E_n)} \\
+ \sum_{m \neq v} \sum_{n \neq v} \frac{\langle w | z | n \rangle \langle n | H^{(1)} | m \rangle \langle m | H^{(hf)} | v \rangle}{(E_v - E_m)(E_v - E_n)} + \sum_{m \neq v} \sum_{n \neq v} \frac{\langle w | z | n \rangle \langle n | H^{(hf)} | m \rangle \langle m | H^{(1)} | v \rangle}{(E_v - E_m)(E_v - E_n)} \\
- \langle w | H^{(hf)} | w \rangle \sum_{m \neq w} \frac{\langle w | H^{(1)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)^2} - \sum_{n \neq v} \frac{\langle w | z | n \rangle \langle n | H^{(1)} | v \rangle}{(E_v - E_n)^2} \langle v | H^{(hf)} | v \rangle,
\]
### Nuclear Anapole Moment: Summary

<table>
<thead>
<tr>
<th>Group</th>
<th>$\kappa$</th>
<th>$\kappa_2$</th>
<th>$\kappa_{hf}$</th>
<th>$\kappa_\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Johnson et al. [1]</td>
<td>0.117(16)</td>
<td>0.0140</td>
<td>0.0049</td>
<td>0.098(16)</td>
</tr>
<tr>
<td>Haxton et al. [2]</td>
<td>0.112(16)</td>
<td>0.0140</td>
<td>0.0078</td>
<td>0.090(16)</td>
</tr>
<tr>
<td>Flambaum and Murray [3]</td>
<td>0.112(16)</td>
<td>0.0111</td>
<td>0.0071</td>
<td>0.092(16)</td>
</tr>
<tr>
<td>Bouchiat and Piketty [4]</td>
<td>0.0084</td>
<td>0.0078</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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 $^{133}\text{Cs}$ 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**

Electric-dipole matrix elements

\[
E^{(2a)}_{\text{PNC}} = A_1 \sum_{j \neq v} \langle 7S | z | j \rangle \langle j | H^{(2a)}_{\text{PNC}} | 6S \rangle - A_2 \sum_{j \neq w} \langle 7S | H^{(2a)}_{\text{PNC}} | j \rangle \langle j | z | 6S \rangle
\]

PNC matrix elements

Fist four terms in the sums are replaced by all-order matrix elements

Same accuracy is expected as spin-independent PNC
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!!*

THEORY: HOW TO CALCULATE PNC AND DIPOLE MATRIX ELEMENTS?
• Configuration interaction (CI)
• Many-body perturbation theory
• Relativistic all-order method (coupled-cluster)
• Perturbation theory in the screened Coulomb interaction (PTSCl), 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
**RELATIVISTIC ALL-ORDER METHOD**

This image contains a periodic table of elements with annotations such as "Singly-ionized ions" and "Ground-state Configuration." The table includes columns for atomic number, symbol, name, atomic weight, ground-state configuration, and ionization energy (in eV). It also highlights different elements and provides a legend for various properties such as solids, liquids, gases, and artificially prepared substances.
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
Cesium: atom with single (valence) electron outside a closed core.

\[ \text{Cs} \quad Z=55 \]
Cs: atom with single (valence) electron outside of a closed core.

\[ |\Psi_v^{(0)}\rangle = a_v^\dagger |\Psi_{\text{core}}\rangle \]

Core wave function

Creation operator for state \( v \)

Lowest-order wave function

Core
Lowest order

Core

Single-particle excitations

Double-particle excitations

ALL-ORDER ATOMIC WAVE FUNCTION (SD)

- core
- valence electron
- any excited orbital
**ALL-ORDER ATOMIC WAVE FUNCTION (SD)**

- **Lowest order**
  
  \[ | \Psi^{(0)}_V \rangle \]

- **Core**

- **Valence electron**

- **Any excited orbital**

- **Single-particle excitations**

  \[
  \sum_{ma} \rho_{ma} a_m^\dagger a_a | \Psi^{(0)}_V \rangle
  \]

  \[
  \sum_{m \neq v} \rho_{mv} a_m^\dagger a_v | \Psi^{(0)}_V \rangle
  \]

- **Double-particle excitations**

  \[
  \frac{1}{2} \sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a | \Psi^{(0)}_V \rangle
  \]

  \[
  \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_a a_v | \Psi^{(0)}_V \rangle
  \]
There are some many of equations!

\[ \rho_{mnab} \]

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 \( \rho_{mnab} \): it is a really large file!
These are really complicated equations!!!

• “Quadruple” term:

\[
\sum_{rs} g_{mnrs} \rho_{rsab}
\]

Indices \(mnrs\) can be ANY orbitals

Basis set: \(n_{\text{max}} = 35, l_{\text{max}} = 6\)

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

• Program has to be exceptionally efficient!
All-order method: Correlation correction to ground state energies of alkali-metal atoms
So we calculated all $\rho_{ma}$, $\rho_{mnab}$, $\rho_{mv}$, $\rho_{mnva}$.

We now have a really large file with $\rho$.

How do we calculate $E_1$ and PNC matrix elements?

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

$Z_{wv}^{(0)} + Z_{wv}^{(a)} + \ldots + Z_{wv}^{(t)}$
### RESULTS FOR ALKALI–METAL ATOMS: E1 MATRIX ELEMENTS

<table>
<thead>
<tr>
<th></th>
<th>Na</th>
<th>K</th>
<th>Rb</th>
<th>Cs</th>
<th>Fr</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3p(_{1/2})-3s</td>
<td>4p(_{1/2})-4s</td>
<td>5p(_{1/2})-5s</td>
<td>6p(_{1/2})-6s</td>
<td>7p(_{1/2})-7s</td>
</tr>
<tr>
<td>All-order</td>
<td>3.531</td>
<td>4.098</td>
<td>4.221</td>
<td>4.478</td>
<td>4.256</td>
</tr>
<tr>
<td>Experiment</td>
<td>3.5246(23)</td>
<td>4.102(5)</td>
<td>4.231(3)</td>
<td>4.489(6)</td>
<td>4.277(8)</td>
</tr>
<tr>
<td>Difference</td>
<td>0.18%</td>
<td>0.1%</td>
<td>0.24%</td>
<td>0.24%</td>
<td>0.5%</td>
</tr>
</tbody>
</table>


Add more terms to the all order wave-function

Non-linear terms

Triple excitations

Study the effects of these terms

- Improve accuracy of atomic properties
- Study fundamental symmetries
- Better all-order excitation coefficients
- CI + all-order method
\[ |\Psi_v\rangle = \exp(S)|\Psi_v^{(0)}\rangle \rightarrow \text{DHF wave function} \]

\[ \exp(S_1 + S_2) \]

**COUPLED-CLUSTER METHOD (CCSD)**

- **Core excitation**
- **Valence excitation**
- **Core - Valence excitations**
\[ \exp(S_1 + S_2) = 1 + (S_1 + S_2) + \frac{1}{2!} (S_1 + S_2)^2 + \frac{1}{3!} (S_1 + S_2)^3 + \frac{1}{4!} (S_1 + S_2)^4 + \ldots \]

SIX TERMS ONLY!

Linear part

Non-linear part

\[ \frac{1}{2} (S_1^2 + 2S_1S_2 + S_2^2) + \frac{1}{6} (S_1^3 + 3S_1^2S_2) + \frac{1}{24} S_1^4 \]
NON-LINEAR TERMS

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

800 TERMS!
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

\[
\sum_{mn rab} \sum_{ijkl} g_{ijkl} \rho_{mnr v ab} : a_i^\dagger a_j^\dagger a_k : : a_m^\dagger a_n^\dagger a_r^\dagger a_b a_a a_v : \left| \Psi^{(0)}_v \right> 
\]

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

Problem: too many excitation coefficients $\rho_{mnrvab}$.
Triple excitations

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

Doubles:

Cs: $a,b = 1s^22s^22p^63s^23p^63d^104s^24p^64d^{10}5s^25p^6$

$m,n : finite basis set = (35 \times 13) \times (35 \times 13)$

Smallest required basis set:
Need total about 300 MB (+extra 150MB file)

Extra index $r$ gives at least a factor $(35 \times 13) : over 130 GB$!

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!
Add more terms to the all order wave-function

Non-linear terms

Non-linear terms:  
R. Pal, M.S. Safronova, W.R. Johnson, A. Derevianko, S. G. Porsev,  

Triple excitations

Triple excitations:  
E. Iskrenova-Tchoukova and M.S. Safronova, in progress
• Configuration interaction (CI)
• Many-body perturbation theory
• Relativistic all-order method (coupled-cluster)
• Perturbation theory in the screened Coulomb interaction (PTSCl), all-order approach

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

*under development
\[ \Psi = \sum_{i} c_i \Phi_i \quad \text{Single-electron valence basis states} \]

\[ \left( H^{\text{eff}} - E \right) \Psi = 0 \]

Example: two particle system:

\[ H^{\text{eff}} = h_1(r_1) + h_1(r_2) + h_2(r_1, r_2) \]

\[ \frac{1}{|r_1 - r_2|} \]
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.
$H_{\text{eff}}$ is modified using perturbation theory expressions

$$h_1 \rightarrow h_1 + \Sigma_1$$

$$h_2 \rightarrow h_2 + \Sigma_2$$

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

$\Sigma_1, \Sigma_2$ are obtained using perturbation theory

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

\begin{align*}
(\Sigma_1)_{mn} &= (\tilde{\varepsilon}_n - \varepsilon_m)\rho_{mn} \\
(\Sigma_2)^L_{mnkl} &= (\tilde{\varepsilon}_k + \tilde{\varepsilon}_l - \varepsilon_m - \varepsilon_n)\rho^L_{mnkl}
\end{align*}

Advantages: most complete treatment of the correlations and applicable for many-valence electron systems
# CI + ALL-ORDER: PRELIMINARY RESULTS

<table>
<thead>
<tr>
<th></th>
<th>Experiment</th>
<th>CI</th>
<th>DIF</th>
<th>CI+II</th>
<th>DIF</th>
<th>CI+ALL</th>
<th>DIF</th>
</tr>
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<tbody>
<tr>
<td><strong>IP</strong></td>
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<td>266</td>
<td>182848</td>
<td>91</td>
</tr>
<tr>
<td><strong>3s3p 3P</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
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### Ionization potentials

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