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


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

Weak charge $Q_W$

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
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

Parity Violation

Atomic Clocks

Structure within the Atom

Quark
Size < 10^{-19} m

Nucleus
Size ~ 10^{-14} m

Electron
Size < 10^{-19} m

Neutron and Proton
Size ~ 10^{-15} m

Atom
Size ~ 10^{-10} m

If the protons and neutrons in this picture were 10 cm across, then the quarks and electrons would be less than 0.1 m, in size and the entire atom would be about 19 km across.

NEED ATOMIC PROPERTIES

Quantum information

P_{1/2}

D_{5/2}

S_{1/2}

"quantum bit"
ATOMIC PROPERTIES

- Magic wavelength
- Parity nonconserving amplitudes
- Derived: Weak charge $Q_w$, Anapole moment
- Line strengths
- Oscillator strengths
- ac and dc Polarizabilities
- Isotope shifts
- Hyperfine constants
- Energies
- BBR shifts
- van der Waals coefficients
- Electron electric-dipole moment enhancement factors
- Fine-structure intervals
- Branching ratios
- Atom-wall interaction constants
- Transition probabilities
- Lifetimes
- Energies
- Wavelengths
- Ac and dc Polarizabilities
- Parity nonconserving amplitudes
- and others...
- Oscillator strengths
- Branching ratios
- Atom-wall interaction constants
- Oscillator strengths
- Parity nonconserving amplitudes
- and others...
HOW TO ACCURATELY CALCULATE ATOMIC PROPERTIES?

Very precise calculation of atomic properties

We also need to evaluate uncertainties of theoretical values!
EXPERIMENTAL PNC STUDIES
# Experimental PNC Studies

<table>
<thead>
<tr>
<th>Element</th>
<th>Mass Number</th>
<th>Ground State</th>
<th>Name</th>
<th>Ground-State Energy (eV)</th>
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<tbody>
<tr>
<td>Ce</td>
<td>140</td>
<td>58</td>
<td>Cerium</td>
<td>236.956</td>
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<tr>
<td>Ba</td>
<td>137</td>
<td>56</td>
<td>Barium</td>
<td>390.82</td>
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<tr>
<td>Fr</td>
<td>223</td>
<td>88</td>
<td>Francium</td>
<td>793.19</td>
</tr>
</tbody>
</table>

*Based upon $^{12}$C. () 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)


Stark interference scheme to measure ratio of the PNC amplitude and the Stark-induced amplitude $\beta$

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

NUCLEAR SPIN-INDEPENDENT PNC

Average of 1 & 2

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

Weak Charge \( Q_W \)

NUCLEAR SPIN-DEPENDENT PNC

Difference of 1 & 2

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

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

**THEORY INPUT**

**Weak Charge** $Q_w$

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

Need theory calculation in terms of $Q_w$

Need $\beta$

**Nuclear anapole moment**

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

Need theory calculation in terms of anapole moment

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

Electric-dipole matrix elements

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

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

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

\( \gamma_5 \) - Dirac matrix
Tensor transition polarizability $\beta$ can be calculated from electric-dipole matrix elements and corresponding energies.

Theory recommended value [1]: $27.11(22) a^3_0$

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

New measurement of 6s-7p matrix elements [2]: $27.22(11) a^3_0$

Measured value (from $M_{1\text{HFS}} / \beta$) [3]: $27.02(8) a^3_0$

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.
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
**DETERMINATION OF \( Q_W \)**

Wood et al. (1997) \( \text{Im}(E_{PNC})/\beta \)  
Bennett & Wieman (1999)  
Measurement of \( \beta \)  
Derevianko (2000,2002)  
Calculation of Breit correction  
Dzuba et al. (2000)  
Calculation of Breit correction  
Kozlov et al. (2001)  
Calculation of \( E_{PNC} \), Breit correction  
Johnson et al. (2001)  
Calculation of vacuum pol. corr.  
Milstein & Sushkov (2002)  
Calculation of vacuum pol. corr.  
Vasilyev et al. (2002)  
Measurement of 6s-7p trans., \( \beta \)  
Dzuba et al. (2002) \( E_{PNC} \)  
Flambaum & Kuchiev (2002)  
Milstein et al. (2003)  
self-energy & vertex corr.

<table>
<thead>
<tr>
<th>( E_{PNC} )</th>
<th>Expt</th>
<th>Theor</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>-72.11(27)</td>
<td></td>
<td></td>
<td>1( \sigma )</td>
</tr>
<tr>
<td>-72.06(28)</td>
<td></td>
<td></td>
<td>2.5( \sigma )</td>
</tr>
<tr>
<td>-72.61(28)</td>
<td></td>
<td></td>
<td>1.3( \sigma )/0.7( \sigma )</td>
</tr>
<tr>
<td>-72.42(28)</td>
<td></td>
<td></td>
<td>1.5( \sigma )/no dev.</td>
</tr>
<tr>
<td>-72.5(7)</td>
<td></td>
<td></td>
<td>no deviation</td>
</tr>
<tr>
<td>-72.12(28)</td>
<td></td>
<td></td>
<td>2.2( \sigma )/1.2( \sigma )</td>
</tr>
<tr>
<td>-72.65(49)</td>
<td></td>
<td></td>
<td>1.1( \sigma )</td>
</tr>
<tr>
<td>-72.16(29)</td>
<td></td>
<td></td>
<td>2( \sigma )</td>
</tr>
<tr>
<td>-72.71(29)</td>
<td></td>
<td></td>
<td>no deviation</td>
</tr>
<tr>
<td>-72.81(28)</td>
<td></td>
<td></td>
<td>0.6( \sigma )</td>
</tr>
</tbody>
</table>
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?**

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

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

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

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

**MORE SPIN-DEPENDENT PNC EFFECTS**

\[ \kappa = \kappa_a + \kappa_2 + \kappa_{hf} \]

\((V_e, A_N)\) 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 \(\kappa_{hf}\) can be calculated.

ANAPOLE MOMENT AND AXIAL-VECTOR TERMS

\[ E_{\text{PNC}}^{(2,a)} = A_1 \sum_{j \neq v} \langle w || z || j \rangle \langle j || H_{\text{PNC}}^{(2,a)} || v \rangle \varepsilon_v - \varepsilon_j + A_2 \sum_{j \neq w} \langle w || H_{\text{PNC}}^{(2,a)} || j \rangle \langle j || z || v \rangle \varepsilon_w - \varepsilon_j \]

Electric-dipole matrix elements

PNC matrix elements

Angular momentum coefficients

\[ H_{\text{PNC}}^{(2,a)} = \frac{G_F}{\sqrt{2}} K_i \alpha \beta \rho_v(r), \quad i = 2, a \]
\[ \langle w | IF_1 M_1 | z | v | IF_1 M_1 \rangle^{(hf)} = \sum_{m \neq w} \frac{\langle w | H^{(1)} | n \rangle \langle n | H^{(hf)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)(E_w - E_n)} + \sum_{m \neq w} \frac{\langle w | H^{(hf)} | n \rangle \langle n | H^{(1)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)(E_w - E_n)} + \sum_{m \neq w} \frac{\langle w | H^{(1)} | m \rangle \langle m | z | n \rangle \langle n | H^{(hf)} | v \rangle}{(E_w - E_m)(E_v - E_n)} + \sum_{m \neq n} \frac{\langle w | H^{(hf)} | m \rangle \langle m | z | n \rangle \langle n | H^{(1)} | v \rangle}{(E_w - E_m)(E_v - E_n)} + \sum_{m \neq n} \frac{\langle w | z | n \rangle \langle n | H^{(1)} | m \rangle \langle m | H^{(hf)} | v \rangle}{(E_v - E_m)(E_v - E_n)} + \sum_{m \neq n} \frac{\langle w | z | n \rangle \langle n | H^{(hf)} | m \rangle \langle m | H^{(1)} | v \rangle}{(E_v - E_m)(E_v - E_n)} + \sum_{m \neq w} \frac{\langle w | H^{(hf)} | w \rangle \sum_{m \neq w} \langle w | H^{(1)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)^2} - \sum_{n \neq v} \frac{\langle w | z | n \rangle \langle n | H^{(1)} | v \rangle}{(E_v - E_n)^2} \langle v | H^{(hf)} | v \rangle, \]
<table>
<thead>
<tr>
<th>Group</th>
<th>$\kappa$</th>
<th>$\kappa_2$</th>
<th>$\kappa_{hf}$</th>
<th>$\kappa_a$</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 $^{133}$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

\[ E_{\text{PNC}}^{(2a)} = A_1 \sum_{j \neq v} \left\langle 7s \mid z \mid j \right\rangle \left\langle j \left| H_{\text{PNC}}^{(2a)} \right| 6s \right\rangle \varepsilon_{6s} - \varepsilon_j + A_2 \sum_{j \neq w} \left\langle 7s \left| H_{\text{PNC}}^{(2a)} \right| j \right\rangle \left\langle j \mid z \mid 6s \right\rangle \varepsilon_{7s} - \varepsilon_j \]

Electric-dipole matrix elements

PNC matrix elements

First 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.

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 (PTSCl), 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**

Singly-ionized ions
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.

Cs  Z=55

Core  $1s^2...5p^6$  6s  valence electron

Valence electron

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

\[ |\Psi^{(0)}_v\rangle = a^\dagger_v |\Psi_{\text{core}}\rangle \]
Lowest order  

Core  

Single-particle excitations  

Double-particle excitations  

- Core  
- Valence electron  
- Any excited orbital  

ALL-ORDER ATOMIC WAVE FUNCTION (SD)
ALL-ORDER ATOMIC WAVE FUNCTION (SD)

Lowest order

Core

\[ |\Psi_v^{(0)}\rangle \]

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

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

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

\( \rho_{mnab} \)  

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

\( m, n : \text{finite basis set} = (35 \times 13) \times (35 \times 13) \)

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 E1 and PNC matrix elements?**

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

\[
z_{wv}^{(0)} + z^{(a)} + \ldots + z^{(t)}
\]
**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 this terms
- Improve accuracy of atomic properties
- Study fundamental symmetries
- Better all-order excitation coefficients

CI + all-order method
COUPLED-CLUSTER METHOD (CCSD)

\[ |\Psi_v\rangle = \exp(S)|\Psi_v^{(0)}\rangle \rightarrow \text{DHF wave function} \]

\[ \exp(S_1 + S_2) \]

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

Linear part

Non-linear part

SIX TERMS ONLY!

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

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

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

\[ \sum_{mnrab} \rho_{mnrvab} a_m^\dagger a_n^\dagger a_r a_a a_b a_v \left| \Psi_v^{(0)} \right> \]

**Problem:** too many excitation coefficients \( \rho_{mnrvab} \).
Triple excitations

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

Doubles:

$$\rho_{mnab}$$

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

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

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

Triple excitations

Non-linear terms:

Triple excitations:
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)
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• Configuration interaction + second-order MBPT
• Configuration interaction + all-order methods*

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

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

Example: two particle system:

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

\[
\frac{1}{|r_1 - r_2|}
\]

\[
\text{one–body part} \quad \text{two–body part}
\]
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

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

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

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

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

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<th>CI+II</th>
<th>DIF</th>
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### Ionization potentials

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<tr>
<td>Ba</td>
<td>-6.4%</td>
<td>1.7%</td>
<td>0.5%</td>
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</table>

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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