A Symposium on Atomic Physics: A Tribute to Walter Johnson

Applications of the All-Order Method: From Parity Violation to Atomic Clocks

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Relativistic all-order equations for helium

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The ground-state energy of helium is calculated to all orders in perturbation theory starting from a relativistic “no-pair” many-body Hamiltonian in which contributions of virtual electron-positron pairs are ignored. In this calculation only Coulomb interactions between the electrons are considered. Two all-order calculations are presented: one calculation is based on nuclear Coulomb-field orbitals and the second is based on Hartree-Fock orbitals. For each calculation the all-order equations of many-body perturbation theory are solved iteratively. The resulting numerical value for the ground-state energy from the Coulomb-field calculation is $-2.903 \, 856(1)$ a.u., while the Hartree-Fock calculation gives $-2.903 \, 855(2)$ a.u. Both of these values agree with that obtained by correcting the well-established nonrelativistic energy for lowest-order relativistic effects.
Benchmark problems for understanding of atomic properties: Tests of theory and experiment
**Parity violation studies with heavy atoms**

**MOTIVATION: PNC**

Parity non-conservation (PNC) studies are crucial in understanding fundamental symmetries in physics. PNC violations can provide insights into the Standard Model and beyond, particularly in the context of heavy atoms where the effects are more pronounced due to the increased quantum numbers.

### Properties of the Interactions

<table>
<thead>
<tr>
<th>Property</th>
<th>Interaction</th>
<th>Gravitational</th>
<th>Weak (Electroweak)</th>
<th>Electromagnetic</th>
<th>Strong</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acts on:</td>
<td>Mass – Energy</td>
<td>Flavor</td>
<td>Electric Charge</td>
<td>Color Charge</td>
<td></td>
</tr>
<tr>
<td>Particles experiencing:</td>
<td>All</td>
<td>Quarks, Leptons</td>
<td>Electrically charged</td>
<td>Quarks, Gluons</td>
<td></td>
</tr>
<tr>
<td>Particles mediating:</td>
<td>Graviton (not yet observed)</td>
<td>W⁺ W⁻ Z⁰</td>
<td>γ</td>
<td>Gluons</td>
<td>Hadrons</td>
</tr>
<tr>
<td>Strength relative to electromag</td>
<td>10⁻¹⁸ m</td>
<td>0.8</td>
<td>1</td>
<td>25</td>
<td></td>
</tr>
<tr>
<td>for two u quarks at:</td>
<td>10⁻⁴¹</td>
<td>10⁻⁴</td>
<td>1</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>for two protons in nucleus</td>
<td>3 × 10⁻¹⁷ m</td>
<td>10⁻⁷</td>
<td>1</td>
<td>Not applicable to quarks</td>
<td>20</td>
</tr>
</tbody>
</table>

**Resources:**

- [http://CPEPweb.org](http://CPEPweb.org)
- Cs experiment, University of Colorado
Correlation correction to ground state energies of alkali-metal atoms

Why all-order?

Correlation energy (cm⁻¹) vs. Nuclear charge Z

- Second order: 4 terms
- Third order: 56 terms

Graph showing correlation energy for Na, K, Rb, Cs, and Fr.
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 useful for particular problems

\[ H |\Psi_v\rangle = E |\Psi_v\rangle \]
RELATIVISTIC ALL-ORDER METHOD

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

Scheme:

1. Calculate the atomic wave functions and energies
2. Calculate various matrix elements
3. Calculate “derived” properties such as PNC amplitudes
Cs: atom with single (valence) electron outside of a closed core.

Lowest-order atomic wave function

\[ \Psi_v^{(0)} = \hat{a}_v \Psi_{\text{core}} \]
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**

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

\[ \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_a a_v |\Psi_v^{(0)}\rangle \]
The derivation gets **really complicated** if you add triples!

Solution: **develop analytical codes** that do all the work for you!

**Input:** ASCII input of terms of the type

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

**Output:** final simplified formula in LATEX to be used in the all-order equation
PROBLEM A WITH EQUATIONS:
There are some many of them !!!

\[ \rho_{mnab} \]

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!
PROBLEM B WITH EQUATIONS:
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!

Actual implementation: Problem 3

$a,b$ core (17 shells)
Correlation correction to ground state energies of alkali-metal atoms

### RESULTS FOR ALKALI–METAL ATOMS: E1 MATRIX ELEMENTS

<table>
<thead>
<tr>
<th></th>
<th>Na 3p&lt;sub&gt;1/2&lt;/sub&gt;-3s</th>
<th>K 4p&lt;sub&gt;1/2&lt;/sub&gt;-4s</th>
<th>Rb 5p&lt;sub&gt;1/2&lt;/sub&gt;-5s</th>
<th>Cs 6p&lt;sub&gt;1/2&lt;/sub&gt;-6s</th>
<th>Fr 7p&lt;sub&gt;1/2&lt;/sub&gt;-7s</th>
</tr>
</thead>
<tbody>
<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>


**Cs**: R.J. Rafac et al., Phys. Rev. A 60, 3648 (1999),


ATOMIC PROPERTIES

- Energies
- Wavelengths
- Branching ratios
- Atom-wall interaction constants
- Oscillator strengths
- Line strengths
- Parity nonconserving amplitudes
- Hyperfine constants
- Isotope shifts
- Transition probabilities
- Energies
- BBR shifts
- van der Waals coefficients
- Electron electric-dipole moment enhancement factors
- Fine-structure intervals

Derived:
- Magic wavelength
- BBR shifts
- Weak charge $Q_w$
- Anapole moment
- Parity nonconserving amplitudes
- Hyperfine constants
- Oscillator strengths
- Line strengths
- Isotope shifts
- Transition probabilities
- Energies
- BBR shifts
- van der Waals coefficients
- Electron electric-dipole moment enhancement factors
- Fine-structure intervals

and others ...

...
Quantum communication, cryptography and quantum information processing

Need calculations of atomic properties


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
Non-linear terms

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

800 terms!
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!
Singly-ionized ions
FUTURE WORK:
CONFIGURATION INTERACTION
+
ALL-ORDER METHOD

*under development
CI works for systems with many valence electrons but cannot accurately account for core-valence and core-core correlations.

All-order method cannot accurately describe valence-valence correlation.

Therefore, two methods are combined to acquire benefits from both approaches.
### CI + ALL-ORDER: PRELIMINARY RESULTS

<table>
<thead>
<tr>
<th>Mg</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>
</thead>
<tbody>
<tr>
<td>IP</td>
<td>182939</td>
<td>179525</td>
<td>3414</td>
<td>182673</td>
<td>266</td>
<td>182848</td>
<td>91</td>
</tr>
<tr>
<td>3s3p</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J=0</td>
<td>21850</td>
<td>20899</td>
<td>951</td>
<td>21764</td>
<td>86</td>
<td>21824</td>
<td>26</td>
</tr>
<tr>
<td>J=1</td>
<td>21870</td>
<td>20919</td>
<td>951</td>
<td>21785</td>
<td>85</td>
<td>21843</td>
<td>27</td>
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<tr>
<td>J=2</td>
<td>21911</td>
<td>20960</td>
<td>951</td>
<td>21829</td>
<td>82</td>
<td>21888</td>
<td>23</td>
</tr>
<tr>
<td>3s3p</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3P</td>
<td>J=1</td>
<td>35051</td>
<td>34486</td>
<td>565</td>
<td>35048</td>
<td>3</td>
<td>35061</td>
</tr>
<tr>
<td>3P</td>
<td>J=2</td>
<td>41197</td>
<td>40392</td>
<td>805</td>
<td>41110</td>
<td>87</td>
<td>41151</td>
</tr>
<tr>
<td>3s4s</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3S</td>
<td>J=1</td>
<td>43503</td>
<td>42664</td>
<td>839</td>
<td>43428</td>
<td>75</td>
<td>43486</td>
</tr>
<tr>
<td>3s4s</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3S</td>
<td>J=2</td>
<td>46403</td>
<td>45108</td>
<td>1295</td>
<td>46296</td>
<td>107</td>
<td>46367</td>
</tr>
</tbody>
</table>

**Ionization potentials**

<table>
<thead>
<tr>
<th></th>
<th>CI</th>
<th>CI+II</th>
<th>CI+All-order</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca</td>
<td>-4.1%</td>
<td>0.6%</td>
<td>0.3%</td>
</tr>
<tr>
<td>Ba</td>
<td>-6.4%</td>
<td>1.7%</td>
<td>0.5%</td>
</tr>
</tbody>
</table>

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

Atomic Clocks

Future:
New Systems
New Methods,
New Problems

Parity Violation

Quantum information
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