Many body study of $g$ factor of boronlike argon

D.E. Maison, L.V. Skripnikov, D.A. Glazov

11.06.2019
Introduction: motivation and previous results;
Theory: Hartree-Fock-Dirac equations;
Theory: coupled cluster approach;
Results: single-reference and multireference;
Conclusion;
Motivation of $g$-factor consideration

Precise theoretical and experimental investigation of electron and atomic $g$ factors may be:

- reliable test for QED;
- helpful for fundamental constants determination ($\alpha = \frac{e^2}{\hbar c}$, $m_e$);
- necessary for precise nuclear magnetic moments determination;
Previous results

System considered: $^{40}_{18}Ar^{13+} \cdot 1s^22s^22p^1$

- 0.663647 (D.A. Glazov et. al., 2013);
- 0.663728 (S. Verdebout et. al., 2014);
- 0.663899 (J.P. Marques et al., 2016);
Atomic wavefunction is the Slater determinant constructed of one-electron orbitals:

$$
\Psi(x_1, \ldots, x_N) = \begin{vmatrix}
\psi_1(x_1) & \ldots & \psi_1(x_N) \\
\vdots & \ddots & \vdots \\
\psi_N(x_1) & \ldots & \psi_N(x_N)
\end{vmatrix}
$$

$$
\left(\hat{h} + \hat{J} - \hat{K}\right) \psi_i(x) = \varepsilon_i \psi_i(x)
$$
Hamiltonian of many-electron system:

\[ \hat{H}_0 = \sum_i \hat{h}(i) + \sum_{i<j} \frac{e^2}{r_{ij}} + \sum_{i<j} \hat{H}_B(i, j) \]

Breit interelectronic interaction:

\[ \hat{H}_B(i, j) = -\frac{\vec{\alpha}_i \cdot \vec{\alpha}_j}{r_{ij}} + \frac{1}{2} \left( \frac{\vec{\alpha}_i \cdot \vec{\alpha}_j}{r_{ij}} - \frac{(\vec{\alpha}_i \vec{r}_{ij}) (\vec{\alpha}_j \vec{r}_{ij})}{r_{ij}^3} \right) \]

Gaunt

retardation

\[ = -\frac{1}{2} \left( \frac{\vec{\alpha}_i \cdot \vec{\alpha}_j}{r_{ij}} + \frac{(\vec{\alpha}_i \vec{r}_{ij}) (\vec{\alpha}_j \vec{r}_{ij})}{r_{ij}^3} \right) \]
Zeeman Hamiltonian:

\[ \hat{H}_Z = \mu_0 \sum_i [\vec{r}_i \times \vec{\alpha}_i] \cdot \vec{B} \]

Zeeman shift and finite-field approach:

\[ \Delta E^{(1)} = g M_J \mu_0 B \quad \Rightarrow \quad g = \frac{1}{\mu_0 M_J} \left. \frac{\partial E}{\partial B} \right|_{B=0} \]

Estimation of QED correction:

\[ \Delta g_{QED} = \mu_0 \frac{g_e - 2}{2} \sum_i \beta_i \Sigma_{z,i} \]
Coupled cluster approach

Basis of CCA is exponential ansatz of wavefunction:

\[ |\psi\rangle = e^{\hat{T}} |\Phi_0\rangle \]

\(\hat{T}\) is the excitation cluster operator which expansion has terms of different excitation orders:

\[ \hat{T} = \sum_{k=1}^{n} \hat{T}_k, \]

where excitation operators of different orders have structure:

\[ \hat{T}_k = \sum_{b_1 < b_2 ... < b_k; i_1 < i_2 ... < i_k} t_{i_1 i_2 ... i_k} a_{b_1}^+ a_{i_1} a_{b_2}^+ a_{i_2} ... a_{b_k}^+ a_{i_k}, \]
Coupled cluster approach: example

\[
\hat{T}_1 \begin{bmatrix}
\psi_1(x_1) & \ldots & \psi_1(x_N) \\
\vdots & & \vdots \\
\psi_i(x_1) & \ldots & \psi_i(x_N) \\
\vdots & & \vdots \\
\psi_N(x_1) & \ldots & \psi_N(x_N)
\end{bmatrix} = \sum_{i \in \text{occ}} \sum_{b \in \text{virt}} t_i^b \begin{bmatrix}
\psi_1(x_1) & \ldots & \psi_1(x_N) \\
\vdots & & \vdots \\
\psi_b(x_1) & \ldots & \psi_b(x_N) \\
\vdots & & \vdots \\
\psi_N(x_1) & \ldots & \psi_N(x_N)
\end{bmatrix}
\]
Coupled cluster approach

Most popular approximations:

- CCS: $\hat{T} \simeq \hat{T}_1$;
- CCSD: $\hat{T} \simeq \hat{T}_1 + \hat{T}_2$;
- CCSD(T): $\hat{T} \simeq \hat{T}_1 + \hat{T}_2$ for wavefunction and $\hat{T}_3$ for energy at 1\textsuperscript{st} PT order;

In all these cases it is convinient to unite the excitation operators with simipar order:

\[
e^{\hat{T}} \simeq 1 + \left( \hat{T}_1 + \hat{T}_2 + \ldots \right) + \frac{1}{2!} \left( \hat{T}_1 + \hat{T}_2 + \ldots \right)^2 + \ldots = \\
= 1 + \hat{T}_1 + \left( \frac{1}{2} \hat{T}_1^2 + \hat{T}_2 \right) + \left( \frac{1}{3} \hat{T}_1^3 + \hat{T}_1 \hat{T}_2 + \ldots \right) + \ldots
\]
Coupled cluster approach

Schrödinger equation gets form:

\[ \hat{H}\psi = E\psi \quad \Rightarrow \quad e^{-\hat{T}}\hat{H}e^{\hat{T}}\Phi_0 = E\Phi_0 \]

and transforms into nonlinear system with unknown cluster amplitudes \( t_i^a, t_{ij}^{ab} \ldots \) and energy as a spectral parameter.

The next basis sets were used for solution:

- small: 25s—, 15p— and 4d— functions;
- middle: 25s—, 15p— and 9d— functions;
- large: 61s—, 50p—, 33d—, 6f— and 4g— functions;
### Single-reference results

<table>
<thead>
<tr>
<th>Method</th>
<th>$^2P_{1/2}$</th>
<th>$^2P_{3/2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dirac-Fock-Gaunt</td>
<td>0.664797</td>
<td>1.331708</td>
</tr>
<tr>
<td>CCS</td>
<td>0.691488</td>
<td>1.330430</td>
</tr>
<tr>
<td>CCSD</td>
<td>0.664962</td>
<td>1.330711</td>
</tr>
<tr>
<td>CCSD(T)</td>
<td>0.664732</td>
<td>1.331075</td>
</tr>
<tr>
<td>CCSDT</td>
<td>0.664764</td>
<td>1.331602</td>
</tr>
<tr>
<td>CCSDT(Q)</td>
<td>0.664762</td>
<td>1.331603</td>
</tr>
<tr>
<td>CCSDTQ</td>
<td>0.664762</td>
<td>1.331603</td>
</tr>
<tr>
<td>FullCI - CCSDTQ</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
</tbody>
</table>
# Multireference results

<table>
<thead>
<tr>
<th>Method</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>MRmin-CISD</td>
<td>0.664763</td>
</tr>
<tr>
<td>MRmin-CISDT</td>
<td>0.664762</td>
</tr>
<tr>
<td>MRmin-CISDTQ</td>
<td>0.664762</td>
</tr>
<tr>
<td>FullCI - MRmin-CISDTQ</td>
<td>0.000000</td>
</tr>
<tr>
<td>MRsp-CISD</td>
<td>0.664762</td>
</tr>
<tr>
<td>MRsp-CISDT</td>
<td>0.664762</td>
</tr>
<tr>
<td>MRsp-CISDTQ</td>
<td>0.664762</td>
</tr>
<tr>
<td>FullCI - MRsp-CISDTQ</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

**MRmin**: active space = \( \{ 2p_{j=1/2, m=1/2}; 2p_{j=1/2, m=-1/2} \} \)

**MRsp**: active space includes all the 2p-bispinors
### Results

<table>
<thead>
<tr>
<th>Method</th>
<th>$^2P_{1/2}$</th>
<th>$^2P_{3/2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Positive, CCSDTQ</td>
<td>0.664762</td>
<td>1.331603</td>
</tr>
<tr>
<td>Negative, (MP2(S))</td>
<td>-0.000335</td>
<td>-0.000089</td>
</tr>
<tr>
<td>Basis set correction (Coulomb)</td>
<td>-0.000001</td>
<td>-0.000002</td>
</tr>
<tr>
<td>QED estimation</td>
<td>-0.000774</td>
<td>0.000773</td>
</tr>
<tr>
<td>Total</td>
<td>0.663652</td>
<td>1.332286</td>
</tr>
<tr>
<td>Glazov et al.</td>
<td>0.663647(1)</td>
<td>1.332285(3)</td>
</tr>
<tr>
<td>Marques et al.</td>
<td>0.663899(2)</td>
<td>1.332372(1)</td>
</tr>
<tr>
<td>Verdebout et al.</td>
<td>0.663728</td>
<td>1.332365</td>
</tr>
</tbody>
</table>
Conclusion

- $g$-factor value of boronlike argon is calculated;
- Breit interaction consideration for atomic systems is tested; it is planned to apply it for more complicated systems;
- convergence level of coupled cluster approach is estimated.
Thank you for your attention!