Many body study of g factor of boronlike argon

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

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Outline

- 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: ${}^{40}_{18}Ar^{13+}$: $1s^2 2s^2 2p^1$

- 0.663647 (D.A. Glazov et. al., 2013);
- 0.663728 (S. Verdebout et. al., 2014);
- 0.663899 (J.P. Marques et al., 2016);

Hartree-Fock-Dirac equations

Atomic wavefunction is the Slater determinant constructed of one-electron orbitals:

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

$$\left(\hat{h} + \hat{J} - \hat{K}\right) \psi_i(x) = \varepsilon_i \psi_i(x)$$

Theory

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:

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

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

Theory

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:

$$\hat{T}_k = \sum_{b_1<b_2\ldots<b_k;i_1<i_2\ldots<i_k} t_{i_1 i_2 \ldots i_k}^{b_1 b_2 \ldots b_k} a_{b_1}^{+} a_{i_1} a_{b_2}^{+} a_{i_2} \ldots a_{b_k}^{+} a_{i_k},$$

Coupled cluster approach: example

$$\hat{T}_1 \begin{vmatrix} \psi_1(x_1) & \dots & \psi_1(x_N) \\ \vdots & & \vdots \\ \psi_i(x_1) & \dots & \psi_i(x_N) \\ \vdots & & \vdots \\ \psi_N(x_1) & \dots & \psi_N(x_N) \end{vmatrix} = \sum_{\substack{i \in occ \\ b \in virt}} t_i^b \begin{vmatrix} \psi_1(x_1) & \dots & \psi_1(x_N) \\ \vdots & & \vdots \\ \psi_b(x_1) & \dots & \psi_b(x_N) \\ \vdots & & \vdots \\ \psi_N(x_1) & \dots & \psi_N(x_N) \end{vmatrix}$$

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 $1^{\underline{st}}$ PT order;

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

$$e^{\hat{T}} \simeq 1 + \left(\hat{T}_1 + \hat{T}_2 + \dots\right) + \frac{1}{2!}\left(\hat{T}_1 + \hat{T}_2 + \dots\right)^2 + \cdots =$$

$$= 1 + \hat{T}_1 + \left(\frac{1}{2}\hat{T}_1^2 + \hat{T}_2\right) + \left(\frac{1}{3}\hat{T}_1^3 + \hat{T}_1\hat{T}_2 + \dots\right) + \dots$$

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

Method	$^2P_{1/2}$	$^2P_{3/2}$
Dirac-Fock-Gaunt	0.664797	1.331708
CCS	0.691488	1.330430
CCSD	0.664962	1.330711
CCSD(T)	0.664732	1.331075
CCSDT	0.664764	1.331602
CCSDT(Q)	0.664762	1.331603
CCSDTQ	0.664762	1.331603
FullCI - CCSDTQ	0.000000	0.000000

Multireference results

Method	
MRmin-CISD	0.664763
MRmin-CISDT	0.664762
MRmin-CISDTQ	0.664762
FullCI - MRmin-CISDTQ	0.000000
MRsp-CISD	0.664762
MRsp-CISDT	0.664762
MRsp-CISDTQ	0.664762
FullCI - MRsp-CISDTQ	0.000000

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

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

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.

The last slide

Thank you for your attention!