Analysis of relativistic effects for correlation correction in highly charged ions

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Outline

1. Motivation
2. Problem and method
3. Results
4. Conclusions

Highly charged ions

Nucleus + several electrons: $N_e \ll Z$

Nuclear potential: $V_{\rm nucl}(r) = -\dfrac{\alpha Z}{r}$

Electron velocity: $v/c \sim \alpha Z$

Low-Z systems: $\alpha Z \ll 1 \longrightarrow \alpha Z$ expansion

High-Z systems: $\alpha Z \sim 1 \longrightarrow$ all orders in αZ

Why study highly charged ions?

- **Stringent tests of bound-state QED**
  [Shabaev *et al.*, *PRA* (2002); Malyshev *et al.*, *JETPL* (2017)]
- **Electron mass** m_e
  [Sturm *et al.*, *Nature* (2014)]
- **Fine-structure constant** α
  [Yerokhin *et al.*, *PRL* (2016); Shabaev *et al.*, *PRL* (2006)]
- **Nuclear magnetic moments**
  [Quint *et al.*, *PRA* (2008)]
- **Searches for new physics**
  [Debierre *et al.*, *PRA* (2022)]

Bound-electron g factor

In a magnetic field, an atomic level splits according to its angular-momentum projection:

$$\delta E = g\,\mu_{\mathrm{B}}\,m_j\,B.$$

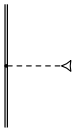
For a highly charged ion,

$$g = g_{\mathrm{D}} + \Delta g_{\mathrm{int}} + \Delta g_{\mathrm{QED}} + \Delta g_{\mathrm{nucl}}$$

This work focuses on the interelectronic correction Δg_{int}.

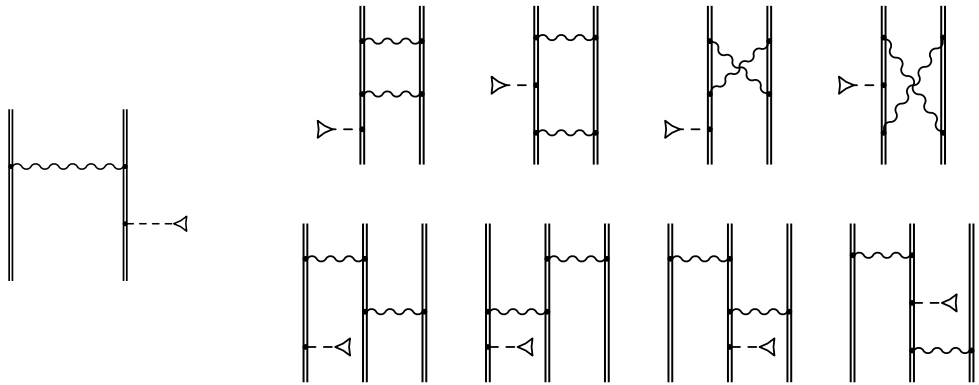
Simple systems
Closed shells + one electron

- H-like: $1s$
- Li-like: $(1s)^2\,2s$
- B-like: $(1s)^2(2s)^2\,2p$



Interaction with an external magnetic field

Interelectronic interaction



$$\Delta g_{\rm int} = \sum_{k\geq 1} \Delta g_{\rm int}^{(k)} = (\alpha Z)^2 \left[\frac{B^{(1)}(\alpha Z)}{Z} + \frac{B^{(2)}(\alpha Z)}{Z^2} + \dots \right]$$

Dirac–Coulomb–Breit model

$$\Lambda_+ H_{\rm DCB} \Lambda_+ |A\rangle = E_A |A\rangle, \qquad H_{\rm DCB} = \sum_j h(j) + \sum_{j<k} V_{\rm Breit}(j,k) - \sum_j V_{\rm scr}(r_j).$$

One-electron Hamiltonian

$$h = c\,\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m_e c^2 + V_{\rm nucl}(r) + V_{\rm scr}(r)$$

Breit interaction operator

$$V_{\rm Breit} = \frac{\alpha}{r_{12}} - \alpha\left(\frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2}{r_{12}} + \frac{1}{2}\left[\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_1, \left[\boldsymbol{\alpha}_2\cdot\boldsymbol{\nabla}_2, r_{12}\right]\right]\right)$$

Screening potentials

Starting effective field: $V_{\rm scr}$

Core–Hartree potential (CH)

$$V_{\rm scr}(r) = \alpha \int_0^\infty dr' \, \frac{\rho_c(r')}{r_>}$$

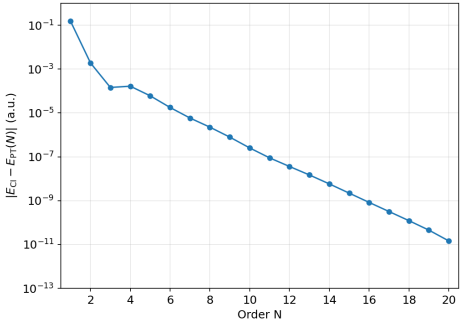
x_α potentials

$$V_{\rm scr}(r) = \alpha \int_0^\infty dr' \, \frac{\rho_t(r')}{r_>} - x_\alpha \, \frac{\alpha}{r} \left(\frac{81}{32\pi^2} \, r \, \rho_t(r) \right)^{1/3}$$

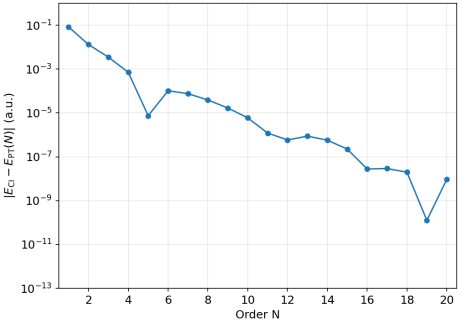
$x_\alpha = 0$	Dirac–Hartree (DH)
$x_\alpha = 2/3$	Kohn–Sham (KS)
$x_\alpha = 1$	Dirac–Slater (DS)

Convergence of PT series to CI value

Ground state: $(1s)^2$

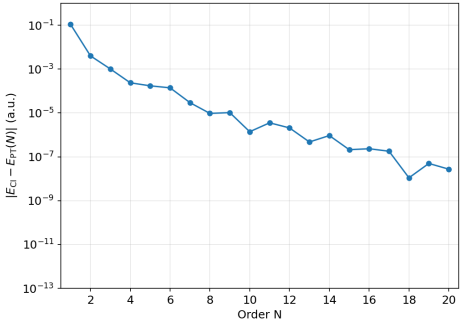


Excited state: $(1s\,2p_{3/2})_{J=2}$

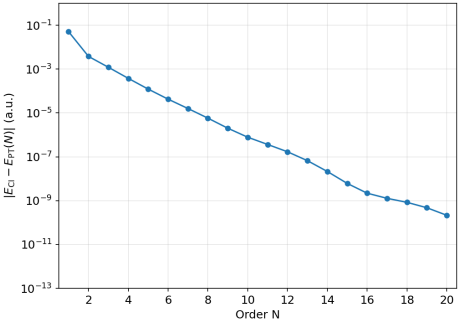


Convergence of PT series to CI value

$(1s\,2s)_{J=0}$

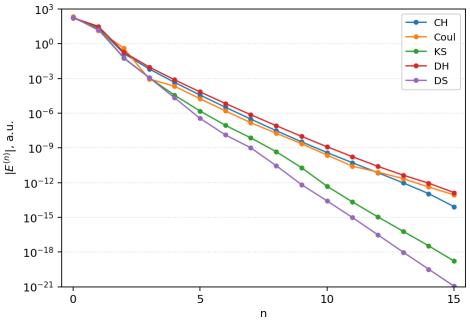


$(1s\,2s)_{J=1}$

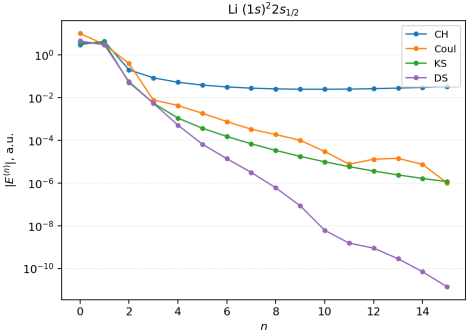


PT convergence. Comparison of screening potentials

Highly charged silicon, $^{28}Si^{11+}$



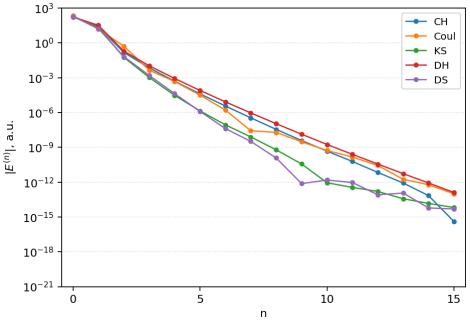
Neutral lithium



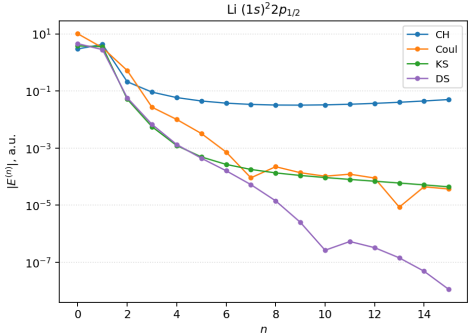
PT convergence. Comparison of screening potentials

$$(1s)^2 2p_{1/2}$$

Lithium-like silicon, Si^{11+}



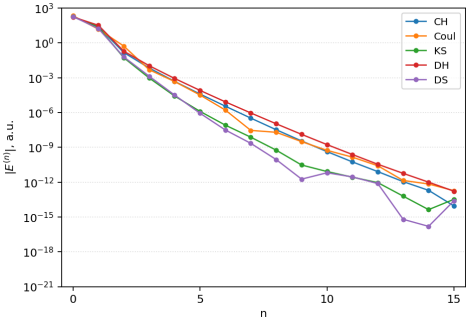
Neutral lithium



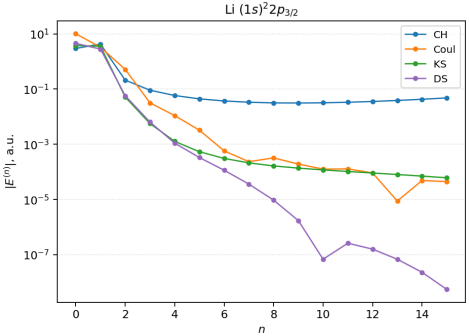
PT convergence. Comparison of screening potentials

$$(1s)^2 2p_{3/2}$$

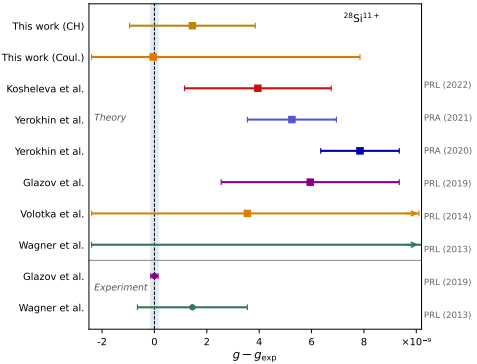
Lithium-like silicon, Si^{11+}



Neutral lithium



The g factor of $^{28}Si^{11+}$ agrees with experiment



Theory	
g^{Coul} **(this work)**	2.000 889 888 4(79)
g^{CH} **(this work)**	2.000 889 889 9(24)
Kosheleva [*PRL* (2022)]	2.000 889 892 4(28)
Yerokhin [*PRA* (2021)]	2.000 889 893 7(17)
Yerokhin [*PRA* (2020)]	2.000 889 896 3(15)
Glazov [*PRL* (2019)]	2.000 889 894 4(34)
Volotka [*PRL* (2014)]	2.000 889 892 0(8)
Wagner [*PRL* (2013)]	2.000 889 909(51)
Experiment	
Glazov [*PRL* (2019)]	2.000 889 888 45(14)
Wagner [*PRL* (2013)]	2.000 889 889 9(21)

Conclusions and outlook

Results

- Developed a software package for calculations in highly charged ions.
- Calculated interelectronic-interaction corrections and studied convergence for different screening potentials.
- The calculated g factor of $^{28}Si^{11+}$ agrees with experiment.

Further work

- Three-photon exchange within rigorous QED
- Inclusion of other contributions
- Further optimization of the software package

Thank you for your attention!

Recursive formulation of perturbation theory

Series expansion in H_1:

$$\tilde{E}_A = \sum_{k=0}^{\infty} E_A^{(k)}, \qquad |\tilde{A}\rangle = \sum_{k=0}^{\infty} \sum_{N} |N\rangle\langle N|A^{(k)}\rangle$$

Recurrence relations:

$$E_A^{(k)} = \sum_M \langle A|H_1|M\rangle\langle M|A^{(k-1)}\rangle - \sum_{j=1}^{k-1} E_A^{(j)} \langle A|A^{(k-j)}\rangle$$

$$\langle N|A^{(k)}\rangle\big|_{N\neq A} = \frac{1}{E_A - E_N}\left[\sum_M \langle N|H_1|M\rangle\langle M|A^{(k-1)}\rangle - \sum_{j=1}^{k-1} E_A^{(j)} \langle N|A^{(k-j)}\rangle\right]$$

$$\langle A|A^{(k)}\rangle = -\tfrac{1}{2} \sum_{j=1}^{k-1} \sum_M \langle A^{(j)}|M\rangle\langle M|A^{(k-j)}\rangle$$

Expansion of g-factor in PT orders

Magnetic operator and energy shift:

$$H_{\rm magn} = \mu_0 \, \mathcal{H} \, U, \quad U = \sum_j [\boldsymbol{\alpha}_j \times \mathbf{r}_j]_z, \quad \Delta E_A = g_A M_A \mu_0 \mathcal{H}$$

Recursive formulas for g-factor corrections:

$$\Delta g_A^{(k)[+]} = \frac{1}{M_A} \sum_{j=0}^{k} \sum_{M,N} \langle A^{(j)} | M \rangle \, \langle M | U | N \rangle \, \langle N | A^{(k-j)} \rangle$$

$$\Delta g_A^{(k)[-]} = \frac{2}{M_A} \sum_{j=0}^{k-1} \sum_{M,N} \sum_{p,n} \frac{\langle p | U | n \rangle}{\varepsilon_p - \varepsilon_n} \, \langle A^{(j)} | M \rangle \, \langle \hat{a}_n^+ \hat{a}_p M | H_1 | N \rangle \, \langle N | A^{(k-j-1)} \rangle$$

The total value of the g factor

g factor in one-electron approximation:

$$g_{\mathrm{D}} = \frac{c}{m_j}\langle a|[\boldsymbol{r}\times\boldsymbol{\alpha}]_z|a\rangle = \frac{2\kappa c}{j(j+1)}\int_0^\infty dr\; r\; G_{n\kappa}(r)F_{n\kappa}(r)$$

g factor of highly charged ions with a spinless nucleus:

$$g = g_{\mathrm{D}} + \Delta g_{\mathrm{int}} + \Delta g_{\mathrm{QED}} + \Delta g_{\mathrm{nucl}}$$

Interelectronic-interaction correction:

$$\Delta g_{\mathrm{int}} = \Delta g_{\mathrm{int}}^{(1)} + \Delta g_{\mathrm{int}}^{(2)} + \ldots = (\alpha Z)^2\left[\frac{1}{Z}B^{(1)}(\alpha Z) + \frac{1}{Z^2}B^{(2)}(\alpha Z) + \ldots\right]$$

Expansion for the parameters $1/Z$ and αZ

$$B^{(i)}(\alpha Z) = b_0^{(i)} + b_2^{(i)}(\alpha Z)^2 + b_4^{(i)}(\alpha Z)^4 + \cdots$$

$$\Delta g_{\text{int}} = \Delta g_{\text{int}}^{(1)}(\alpha Z) + \Delta g_{\text{int}}^{(2)}(\alpha Z) + \Delta g_{\text{int}}^{(3)}(\alpha Z) + \cdots$$

$$\Delta g_{\text{int}}^{(1)}(\alpha Z) = \frac{(\alpha Z)^2}{Z}[b_0^{(1)} + b_2^{(1)}(\alpha Z)^2 + \ldots]$$

$$\Delta g_{\text{int}}^{(2)}(\alpha Z) = \frac{(\alpha Z)^2}{Z^2}[b_0^{(2)} + b_2^{(2)}(\alpha Z)^2 + \ldots]$$

$$\Delta g_{\text{int}}^{(3)}(\alpha Z) = \frac{(\alpha Z)^2}{Z^3}[b_0^{(3)} + b_2^{(3)}(\alpha Z)^2 + \ldots]$$

$$\vdots$$