Nuclear magnetic shielding in boronlike ions

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Motivation

g-factor of highly charged ions

- high-precision ($10^{-9} - 10^{-11}$) measurements and theoretical predictions
- verification of the fundamental theories
- determination of the fundamental constants

Ions with non-zero nuclear spin

- determination of the nuclear magnetic moments from the g-factor investigations

Werth et al., in The Hydrogen Atom (Springer, Berlin, 2001), p. 204,

Quint et al., PRA 78, 032517 (2008),

Yerokhin et al., PRL 107, 043004 (2011).

Zeeman splitting of the hyperfine levels

$$\Delta E(F, M_F) = g_F \mu_0 B M_F$$

$$g_F = g_j \frac{\langle \vec{j}\vec{F} \rangle}{\langle F^2 \rangle} - (1-\sigma)\frac{m_e}{m_p} g_I \frac{\langle \vec{I}\vec{F} \rangle}{\langle F^2 \rangle} + \delta_Q(F)$$

$$g_I = f(g_F, g_j, \sigma, \delta_Q(F))$$

where
g_j — electron g-factor, g_I — nuclear g-factor.

Previous investigations for 1s and 2s states:
Moskovkhin et al., PRA (2004), PRA (2006), PRA (2008),
Yerokhin et al., PRL (2011), PRA (2012).

g-factor correction due to the hyperfine interaction

$$\sigma = \alpha \sum_n \frac{\langle a|W|n\rangle\langle n|U|a\rangle}{E_a - E_n}$$

where

$$W = \frac{[\vec{r} \times \vec{\alpha}]_z}{r^3}, \qquad U = [\vec{r} \times \vec{\alpha}]_z, \qquad \lambda = \mu_0 B \; .$$

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$$\hat{H}|\tilde{a}(\lambda)\rangle = \tilde{E}|\tilde{a}(\lambda)\rangle$$

$$\hat{H} = (\vec{\alpha}\cdot\vec{p}) + \beta m + V(r) + \lambda U$$

$$\sigma = \frac{\alpha}{2} \frac{d}{d\lambda}\bigg|_{\lambda=0} \langle\tilde{a}(\lambda)|W|\tilde{a}(\lambda)\rangle$$

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PT-DKB A-DKB

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PT-DKB method

$$\sigma = \frac{\alpha}{2} \frac{d}{d\lambda}\bigg|_{\lambda=0} \langle \tilde{a}(\lambda)|W|\tilde{a}(\lambda)\rangle$$

$$\hat{H}|a\rangle = E|a\rangle$$

$$\hat{H} = (\vec{\alpha}\cdot\vec{p}) + \beta m + V(\vec{r})$$

$$|a\rangle = \frac{1}{r}\begin{pmatrix} G(r)\Omega_{jlM}(\vec{n}) \\ iF(r)\Omega_{j\bar{l}M}(\vec{n}) \end{pmatrix}$$

$$|\tilde{a}(\lambda)\rangle = |a\rangle + \lambda \sum_n{}' \frac{|n\rangle\langle n|U|n\rangle}{\varepsilon_a - \varepsilon_n}$$

DKB splines: Shabaev et al., PRL 93, 130405 (2004)

where

$$W = \frac{[\vec{r}\times\vec{\alpha}]_z}{r^3}, \qquad U = [\vec{r}\times\vec{\alpha}]_z, \qquad \lambda = \mu_0 B$$

A-DKB method

$$\sigma = \frac{\alpha}{2} \frac{d}{d\lambda}\Big|_{\lambda=0} \langle \tilde{a}(\lambda)|W|\tilde{a}(\lambda)\rangle$$

$$\hat{H}|\tilde{a}(\lambda)\rangle = \tilde{E}|\tilde{a}(\lambda)\rangle$$

$$\hat{H} = (\vec{\alpha}\cdot\vec{p}) + \beta m + V(r) + \lambda U$$

$$|\tilde{a}(\lambda)\rangle = \frac{1}{r}\begin{pmatrix} G_1(r,\theta)e^{i\varphi(M-\frac{1}{2})} \\ G_2(r,\theta)e^{i\varphi(M+\frac{1}{2})} \\ iF_1(r,\theta)e^{i\varphi(M-\frac{1}{2})} \\ iF_2(r,\theta)e^{i\varphi(M+\frac{1}{2})} \end{pmatrix}$$

A-DKB splines: Rozenbaum et al., PRA 89, 012514 (2014)

where

$$W = \frac{[\vec{r}\times\vec{\alpha}]_z}{r^3}, \qquad U = [\vec{r}\times\vec{\alpha}]_z, \qquad \lambda = \mu_0 B$$

Results: $\sigma \times 10^3$

Z	method	$1s$	$2s$	$2p_{1/2}$
6	PT	0.1071	0.0267	24.712
	PT-DKB	0.1071	0.0267	24.712
	A-DKB	0.1071	0.0267	24.717
	Moskovkin	0.1071	0.0267	
16	PT	0.2946	0.0726	9.315
	PT-DKB	0.2946	0.0726	9.315
	A-DKB	0.2948	0.0725	9.325
	Moskovkin	0.2946	0.0726	
32	PT	0.6579	0.1556	4.745
	PT-DKB	0.6579	0.1556	4.745
	A-DKB	0.6591	0.1555	4.748
	Moskovkin	0.6579	0.1556	
83	PT	4.111	0.8363	2.252
	PT-DKB	4.111	0.8363	2.252
	A-DKB	4.109	0.8353	2.252
	Moskovkin	4.111	0.8364	

Volchkova et al., NIMB (2017)

Moskovkin et al., PRA (2004, 2008), Opt. Spectrosc. (2008)

Analitical results for point-like nucleus

$1s$ state:

$$\sigma = \alpha \frac{\alpha Z}{3} S_{1s}(\alpha Z), \qquad S_{1s}(\alpha Z) \approx 1 + \frac{97}{36}(\alpha Z)^2$$

$2s$ state:

$$\sigma = \alpha \frac{\alpha Z}{12} S_{2s}(\alpha Z), \qquad S_{2s}(\alpha Z) \approx 1 + \frac{229}{144}(\alpha Z)^2$$

$2p_{1/2}$ state:

$$\sigma = \alpha \frac{4}{27\alpha Z} S_{2p_{1/2}}(\alpha Z), \qquad S_{2p_{1/2}}(\alpha Z) \approx 1 + \frac{7}{16}(\alpha Z)^2$$

Moore, Mol. Phys. (1999),
Pyper, Mol. Phys. (1999),
Pyper and Zhang, Mol. Phys. (1999).

Results: $\sigma \times 10^3$ for boronlike ions

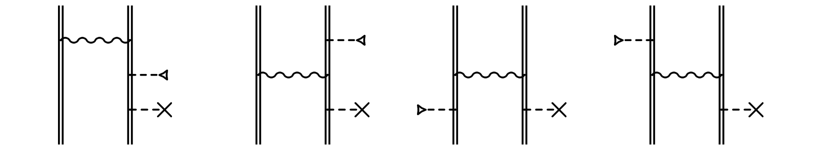
Local screening potential approximately accounts for the interelectronic interaction

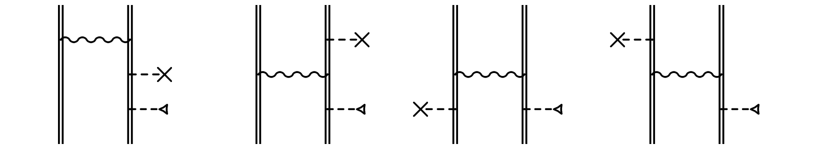
$$V(r) = V_{nucl}(r) + V_{scr}(r)$$

Z	Coulomb	core-Hartree	Kohn-Sham	local Dirac-Fock
6	24.712	33.100	31.177	33.170
16	9.315	10.188	10.028	10.164
32	4.745	4.942	4.907	4.934
82	2.260	2.270	2.268	2.269
83	2.252	2.261	2.259	2.260
92	2.240	2.237	2.238	2.237

Volchkova et al., NIMB (2017)

Electron-electron interaction: one-photon exchange





Results: one-photon exchange for boronlike ions

Calculation within PT-DKB method

Z		Coulomb	core-Hartree	Kohn-Sham
32	$\sigma \times 10^3$	4.7454	4.9421	4.9069
	$\delta_{1\mathrm{ph}}\sigma \times 10^3$	0.3437	0.1562	0.1876
	$(\sigma + \delta_{1\mathrm{ph}}\sigma) \times 10^3$	5.0891	5.0983	5.0945
83	$\sigma \times 10^3$	2.2518	2.2614	2.2593
	$\delta_{1\mathrm{ph}}\sigma \times 10^3$	0.0153	0.0060	0.0077
	$(\sigma + \delta_{1\mathrm{ph}}\sigma) \times 10^3$	2.2671	2.2674	2.2670

Conclusion

1. The g-factor correction due to the hyperfine interaction (nuclear magnetic shielding constant) for the $1s$, $2s$ and $2p_{\frac{1}{2}}$ states has been obtained. The values for the $1s$ and $2s$ states are in agreement with the published results.

2. One-photon-exchange correction to the nuclear magnetic shielding constant has been evaluated for lithium-like ions (in agreement with the published results) and boron-like has been obtained.

3.It is planned to evaluate the contributions of the QED, higher-order interelectronic interaction, and recoil effects.

4. It is planned to investigate the Zeeman splitting of the hyperfine levels for arbitrary magnetic field (Breit-Rabi formula).

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Thank you for attention!