Hyperfine structure calculations in hydrogenlike and heliumlike atoms

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PSAS 24 Zurich

11th June 2024

Hyperfine structure of light atoms

- Interaction of nuclear magnetic moment with that of the electron leads to splitting of energy levels called hyperfine splitting

- It can be measured very accurately and thus represents a good candidate for tests of bound state QED

- Theoreotical results are however severely limited by nuclear effects which cannot be accurately calculated at the moment and contribute already on the 10^{-4} level

- Nuclear effects are typically divided into elastic and inelastic parts
- Elastic effects are expressed in terms of charge and magnetic form factors and represent the dominant hfs nuclear effect, proportional to Zemach radius r_Z
- Dominant inelastic effect is nuclear polarizability and little is known about it due to complexity of its theoretical description
- Nuclear polarizability can be significant, for instance in μD hfs it is supposed to be as large as elastic contribution - for μD there is conflict between theoretical predictions and experimental results

- For electronic atoms the nuclear polarizability effects are much smaller but not negligible
- In the absence of theoretical calculations we determine nuclear polarizability from the comparison with experiment
- Comparing the experimental hfs result with known theoretical results for relativistic and QED effects for the point nucleus together with elastic form factors of nucleus from scattering experiments to extract the nuclear polarizability correction

NRQED method

- For light atoms such as helium the most accurate results are obtained with the nonrelativistic QED (NRQED) method
- Starting point is nonrelativistic few-body Schrodinger equation
- Relativistic and QED effects are accounted for perturbatively with expansion in α and $Z\alpha$
- Energy levels are expressed as a power series

$$E\left(\alpha, \frac{m}{M}\right) = \alpha^2 E^{(2)}\left(\frac{m}{M}\right) + \alpha^4 E^{(4)}\left(\frac{m}{M}\right) + \alpha^5 E^{(5)}\left(\frac{m}{M}\right)$$
$$\alpha^6 E^{(6)}\left(\frac{m}{M}\right) + \alpha^7 E^{(7)}\left(\frac{m}{M}\right) + \cdots$$

- Individual terms can be in turn expanded in powers of electron-to-nucleus mass ratio

$$E^{(i)}\left(\frac{m}{M}\right) = E^{(i,0)} + \frac{m}{M}E^{(i,1)} + \cdots$$

- Individual contributions are obtained as an expectation value of effective operators with nonrelativistic wave function ϕ

- The leading order contribution is expectation value of nonrelativistic Hamiltonian which for helium is

$$E^{(2,0)} \equiv E_0 = \langle H_0 \rangle,\ \ H_0 = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{Z\alpha}{r_1} - \frac{Z\alpha}{r_2} + \frac{\alpha}{r_{12}}$$

- Derivation of higher order effective Hamiltonians is the central problem of NRQED as they became increasingly complicated

- Using NRQED the hyperfine structure effects can be expressed as

$$E_{\mathrm{hfs}} = E_F(1 + \kappa + \delta^{(2)} + \delta^{(3)} + \delta^{(4)} + \delta^{(1)}_{\mathrm{nuc}} + \delta^{(1)}_{\mathrm{rec}} + \delta^{(2)}_{\mathrm{nuc}} + \delta^{(2+)}_{\mathrm{rec}})$$

  where E_F is Fermi splitting and is of the order α^4

- For helium it is

$$E_F = \frac{4\pi Z\alpha}{3mM} g \,\langle \vec{I} \cdot \left[\vec{s}_1\, \delta^3(r_1) + \vec{s}_2\, \delta^3(r_2)\right]\rangle$$

- δ coefficients in different atomic states are strongly correlated and using data from one state (for instance He^+) enables us to improve theoretical prediction in another state (for instance He)

- Nuclear structure contribution is only by a factor α smaller than the leading-order contribution and thus it is significant
- $\delta^{(1)}_{\rm nuc}$ contains two parts, elastic $\delta^{(1)}_{\rm nuc,el}$ and inelastic $\delta^{(1)}_{\rm nuc,inel}$
- Elastic part is proportional to Zemach radius r_Z

$$\begin{aligned}\delta^{(1)}_{\rm nuc,el} &= -2Z\alpha\,\mu\,r_Z,\\ r_Z &= \int d^3r_1\int d^3r_2\,\rho_E(\vec{r}_1)\,\rho_M(\vec{r}_2)\,|\vec{r}_1-\vec{r}_2|\end{aligned}$$

- This can be determined from electron-scattering data, I. Sick, Phys. Rev. C **90**, 064002 (2014)

- Inelastic part $\delta^{(1)}_{\rm nuc,inel}$ cannot be directly calculated so we have to obtain it from the experiment

- We define *effective* Zemach radius $\tilde{r}_Z$ so that

$$\delta^{(1)}_{\rm nuc} = -2Z\alpha\,\mu\,\tilde{r}_Z$$

  which contains both elastic and inelastic parts

- By subtracting r_Z known from electron scattering we obtain the nuclear polarizability contribution

- Alternatively, using $\delta^{(1)}_{\rm nuc}$ determined from one state we improve theoretical prediction for different state

$^3He^+$

- Combining theoretical result for $^3He^+$ with experimental data from A. Schneider et al., Nature (London) **606**, 878 (2022), we get

$$\tilde{r}_Z = 2.600(8)\,\mathrm{fm}$$
$$\tilde{r}_Z - r_Z = 0.072(18)\,\mathrm{fm}$$

Phys. Rev. A **107**, 052802 (2023)

- Surprisingly for helion numerical contribution of nuclear polarizability is only 3%, smaller than for hydrogen

- Obtaining the nuclear structure contribution from He$^+$ enables us to improve accuracy of theoretical prediction for He
- Each δ is split into two parts

$$\delta(\mathrm{He}) = \delta(\mathrm{He}^+) + \delta(\mathrm{He} - \mathrm{He}^+)$$

- $\delta(\mathrm{He}^+)$ is then extracted from experiment A. Schneider et al., Nature (London) **606**, 878 (2022)

Li^{2+}

- In a similar way, using theoretical calculations and experimental data from Li^{+} enables us to obtain theoretical prediction for Li^{2+}

- Our results Phys. Rev. A **108**, 052802 (2023)

$$E_{\rm hfs}(^{6}\mathrm{Li}^{2+}) = 8.479\,190\,(21)\,\mathrm{GHz}$$
$$E_{\rm hfs}(^{7}\mathrm{Li}^{2+}) = 29.855\,013\,(86)\,\mathrm{GHz}$$

- Uncertainty of the result comes exclusively from uncertainty of the experimental Li^{+} hfs result

Hfs calculation in heliumlike atoms

- To improve theoretical prediction for heliumlike atoms we needed to calculate higher-order QED contribution $E^{(7,0)}$
- It is given by a sum of three parts:

$$E^{(7)} = \langle H^{(7)} \rangle + 2 \left\langle H^{(5)} \frac{1}{(E_0 - H_0)'} H^{(4)} \right\rangle + E_L$$

- Calculation of this contribution is very similar to our previous calculation of helium centroid energies of triplet states but much simpler

- On our level of precision we also have to include recoil correction due to hyperfine mixing

$$E_{\mathrm{mix}}^{(6)} = \frac{\langle 2^3 S | V_F | 2^1 S \rangle^2}{E_0(2^3 S) - E_0(2^1 S)}$$

where V_F is Fermi contact interaction, $E_F = \langle V_F \rangle$

- Because the difference in energies in the denominator is small this contribution is significantly enhanced and also higher order corrections to it have to be included

- Contributions to the 2^3S_1 hfs of ^{3}He are

Term	$\times 10^{-6}$	$\times E_F(\mathrm{He})$ [Hz]
$\delta^{(2)}(\mathrm{He\text{-}He}^+)$	3.012 0	−20 279
$\delta^{(2+)}_{\mathrm{rec}}(\mathrm{He\text{-}He}^+)$	−8.993 7 (21)	60 552 (14)
$\delta^{(3)}(\mathrm{He\text{-}He}^+)$	0.184 3	−1 241
$\delta^{(4)}(\mathrm{He\text{-}He}^+)$	0.005 8 (58)	−39 (39)
$\delta(\mathrm{He\text{-}He}^+)$	−5.791 6 (62)	38 993 (41)
$1+\delta(\mathrm{He}^+)$		−6 739 740 174
$\nu_{\mathrm{hfs,theo}}(\mathrm{He})^a$		−6 739 701 181 (41)
$\nu_{\mathrm{hfs,exp}}(\mathrm{He})^b$		−6 739 701 177 (16)

[a] V. Patkóš, V. A. Yerokhin, and K. Pachucki, Phys. Rev. Lett. 131, 183001 (2023);
[b] S. D. Rosner and F. M. Pipkin, Phys. Rev. A **1**, 571 (1970), (E) Phys. Rev. A **3**, 521 (1971);

Li^+

- Our theoretical results can be used also to heliumlike ions such as Li^+ for which enough accurate experimental data is available

- In Li^+ hfs is given by magnetic dipole and electric quadrupole contributions

$$E_{\rm hfs} = A\,\langle \vec{I}\cdot\vec{S}\rangle + B\,\langle (I^i I^j)^{(2)} (S^i S^j)^{(2)}\rangle$$

with symmetric traceless tensors

$$(I^i I^j)^{(2)} = \frac{1}{2}(I^i I^j + I^j I^i) - \frac{\delta^{ij}}{3} I^2$$

- By appropriate combination of experimental transitions it is possible to eliminate quadrupole contribution and obtain $A_{\rm expt}$
- For two isotopes of lithium ion it is

$$A_{\rm exp}(^6{\rm Li}^+) = \frac{1}{6}\,\nu_{0-1} + \frac{5}{12}\,\nu_{1-2}$$
$$A_{\rm exp}(^7{\rm Li}^+) = \frac{1}{6}\,\nu_{1/2-3/2} + \frac{3}{10}\,\nu_{3/2-5/2}$$

where $\nu_{F-F'}$ are the measured $F-F'$ transition energies

- Our theoretical results (Phys. Rev. A. **108**, 052802 (2023)) can be compared with experiment

  W. Sun et al., Phys. Rev. Lett. **131**, 103002 (2023)
  H. Guan et al., Phys. Rev. A **102**, 030801(R) (2020)

  to obtain effective Zemach radius of lithium

System	Reference	$^6\mathrm{Li}$	$^7\mathrm{Li}$
Li^+	Our work	2.39 (2)	3.33 (3)
Li^+	Sun *et al.*	2.44 (2)	
Li^+	Guan *et al.*[a]		3.35 (1)
Li^+	Qi *et al.*[b]	2.40 (16)	3.33 (7)
Li^+	Qi *et al.*[b]	2.47 (8)	3.38 (3)
Li	Puchalski *et al.*[c]	2.29 (4)	3.23 (4)

[a] H. Guan et al., arXiv:2403.06384
[b] X.-Q. Qi et al., Phys. Rev. Lett. **125**, 183002 (2020)
[c] M. Puchalski and K. Pachucki, Phys. Rev. Lett. **111**, 243001 (2013), recalculated for updated nuclear momenta.

- We may also check consistency of theory and experiment in Li and Li^+ by comparing difference of δ calculated and extracted from experiment

Term	$^6\mathrm{Li}$	$^7\mathrm{Li}$
$\delta^{(2)}(\mathrm{Li}\text{-}\mathrm{Li}^+)$	0.000 204 8	0.000 204 8
$\delta^{(2)}_{\mathrm{rec.mix}}(\mathrm{Li}\text{-}\mathrm{Li}^+)$	−0.000 002 4	−0.000 006 2
$\delta^{(3)}(\mathrm{Li}\text{-}\mathrm{Li}^+)$	−0.000 000 5 (47)	−0.000 000 5 (47)
$\delta(\mathrm{Li}\text{-}\mathrm{Li}^+)_{\mathrm{theo}}$	0.000 201 9 (47)	0.000 198 0 (47)
$\delta(\mathrm{Li}\text{-}\mathrm{Li}^+)_{\mathrm{exp}}$ [a,b,c]	0.000 212 9 (24)	0.000 209 5 (29)

[a] W. Sun et al., Phys. Rev. Lett. **131**, 103002 (2023)
[b] H. Guan et al., Phys. Rev. A **102**, 030801(R) (2020)
[c] A. Beckmann, K. D. Böklen, and D. Elke, Z. Phys. 270, 173 (1974).

- Another test of consistency is calculation of ^{6}Li-^{7}Li isotope shift of ground-state hfs

Term	Value
$\delta(^6\mathrm{Li}\text{-}^7\mathrm{Li})_{\mathrm{theo}}$	$-0.000\,000\,1$
$\delta(^6\mathrm{Li}\text{-}^7\mathrm{Li})_{\mathrm{exp}}$	$0.000\,105\,7(5)$
$\delta_{\mathrm{struc}}(^6\mathrm{Li}\text{-}^7\mathrm{Li})$	$0.000\,105\,8(5)$
$\delta_{\mathrm{struc}}(^6\mathrm{Li}^+\text{-}^7\mathrm{Li}^+)$	$0.000\,106\,3(38)$

Summary

- Hyperfine splitting can be used for precise tests of QED
- By extracting nuclear structure contribution from the comparison of experiment and theory in one system we may improve the accuracy of theory in other system
- For He we got excellent agreement with the experiment
- In Li we have confirmed the result that Zemach radius of ^{6}Li is smaller than that of ^{7}Li, despite the fact that for their charge radii the situation is reversed

Thank you for your attention!