Bohr-Weisskopf effect in the thallium atom

S.D. Prosnyak, D.E. Maison, L.V. Skripnikov

Petersburg Nuclear Physics Institute
Quantum Chemistry Laboratory

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Why is this interesting?

- μ is the magnetic moment; $\mathrm{A} = \mathrm{const} \cdot \mu/\mathrm{I}$

  HFS anomaly: ${}^1\Delta^2 = \frac{\mathrm{A}_1 \mu_2 \mathrm{I}_1}{\mathrm{A}_2 \mu_1 \mathrm{I}_2} - 1$

- Information about the nuclei

- Check the accuracy of electronic structure calculations

Nuclear structure corrections

$$\mathrm{A} = (1-\varepsilon)\cdot(1-\delta)\cdot \mathrm{A}_{\mathrm{R_N=0,R_M=0}} + \mathrm{A}_{\mathrm{QED}}$$

- δ - Breit-Rosenthal (Charge distribution)
- ε - Bohr-Weisskopf (Magnetization distribution)
- $\mathrm{A}_{\mathrm{QED}}$ - radiation (Quantum electrodynamics)

Analytic behaviour

Hydrogen-like thallium in the ground state [*].

$$\Delta E = \frac{4}{3}\alpha(\alpha Z)^3 \frac{\mu}{\mu_N} \frac{m}{m_p} \frac{2I+1}{2I} mc^2 \times \big(A(\alpha Z)(1-\delta)(1-\varepsilon) + x_{rad}\big)$$

Analytic behaviour of δ:

$$\delta = \text{const} \cdot R^{2\gamma-1} \text{ , where } \gamma = \sqrt{1-(\alpha Z)^2}$$

*V. M. Shabaev, M. Tomasseli, T. Kühl, A. N. Artemyev, and V. A. Yerokhin, "Ground-state hyperfine splitting of high-Z hydrogen-like ions", Phys. Rev. A, vol 56, no. 1, pp. 62–65, 1997.

Basis set test

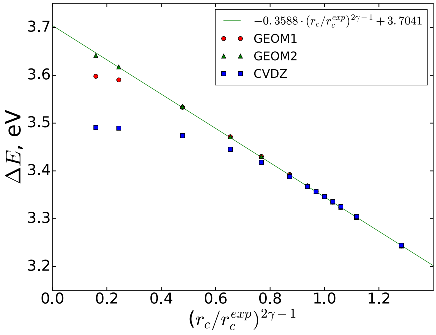


Figure: $\Delta E((r_c/r_c^{exp})^{2\gamma-1})$ for $^{205}Tl^{80+}$, $r_m = 0$.

Extrapolated value of point nucleus ΔE: 3.7041 eV.
Analytic value [Shabaev et al, 1997]: 3.7042 eV.
Thus, gaussian basis set is good for high precision calculation of the HFS constant.

Determining r_m for ^{203}Tl from experimental data for H-like ^{203}Tl

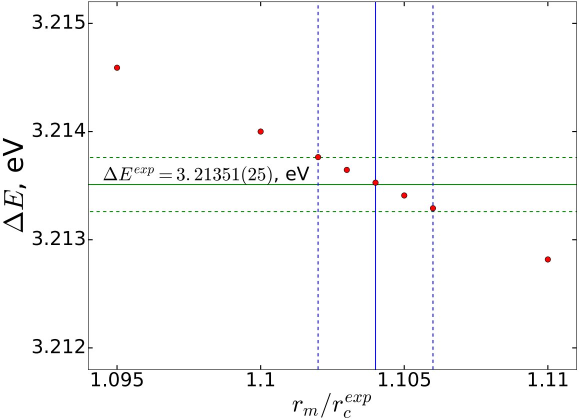


Figure: $\Delta E(r_m/r_c^{exp})$ for $^{203}Tl^{80+}$, $r_c = r_c^{exp}$.

Determining r_m for ^{205}Tl from experimental data for H-like ^{205}Tl

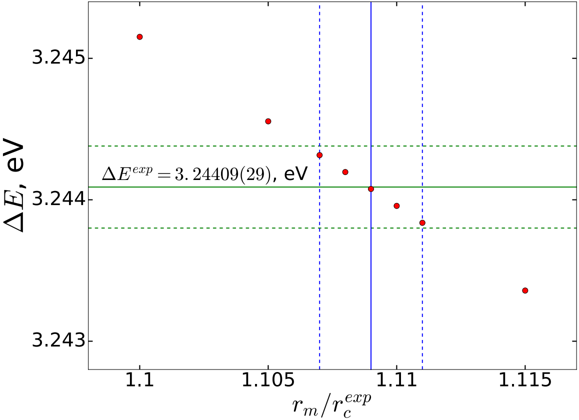


Figure: $\Delta E(r_m/r_c^{exp})$ for $^{205}Tl^{80+}$, $r_c = r_c^{exp}$.

Correlation calculation of the HFS in $6P_{1/2}$ state

r_m/r_c^{exp} is fixed from the data for H-like ^{205}Tl

$^{205}Tl^0$ $6P_{1/2}$ Hyperfine constant A (in MHz).

r_m/r_c^{exp}	0	1	1.1	1.11
HF	18805	18681	18660	18658
CCSD	21965	21807	21781	21778
CCSD(T)	21524	21372	21347	21345
+Basis corr.	-21	-21	-21	-21
+CCSDT-CCSD(T)	+73	+73	+73	+73
+CCSDT(Q)-CCSDT	-5	-5	-5	-5
+Gaunt	-83	-83	-83	-83
Total	21488	21337	21312	21309

$A_{exp} = 21310.835(5)$ MHz

* QED correction is not considered.

Correlation calculation of the HFS in $6P_{1/2}$ state

$^{205}Tl^{0}$ Results review.

Authors	A_p, MHz	ε	A, MHz
Kozlov, 2001	21663	-	-
Safronova, 2005	21390	-	-
Martenson, 1995	21430	0.0061	21300
This work, 2019	21488	0.0084	21309

$$A_{exp} = 21310.835(5) \text{ MHz}$$

Neutral thallium $6P_{3/2}$

r_m/r_c^{exp} is fixed from the data for H-like ^{205}Tl

$^{205}Tl^0$ Hyperfine constant A, MHz.

r_m/r_c^{exp}	0	1	1.1	1.11
HF	1415	1415	1415	1415
CCSD	6	40	46	47
CCSD(T)	244	273	278	278
+Basis corr.	+4	+4	+4	+4
+CCSDT-CCSD(T)	-49	-49	-49	-49
+CCSDT(Q)-CCSDT	+13	+13	+13	+13
+Gaunt	+1	+1	+1	+1
Total	214	243	248	248

$A_{exp} = 265$ MHz

* QED correction is not considered.

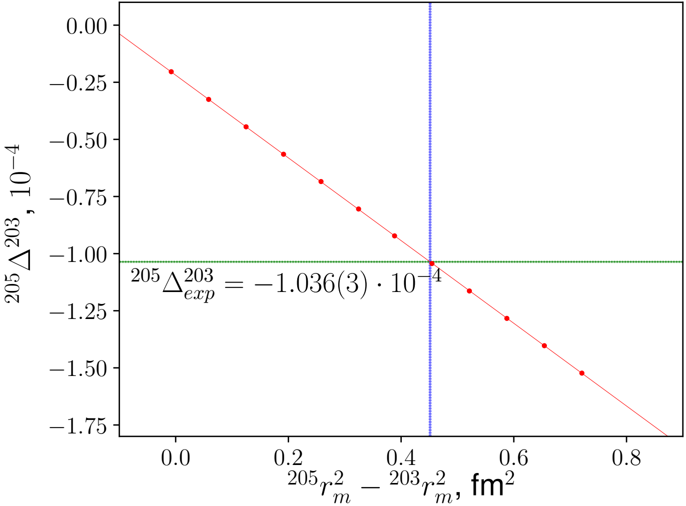
Neutral thallium $6P_{3/2}$

$^{205}Tl^{0}$ Results review.

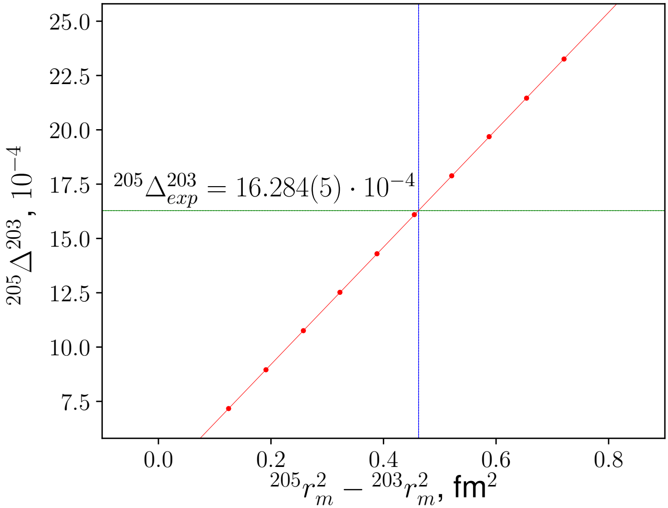
Authors	A_p, MHz	ε	A, MHz
Kozlov, 2001	248	-	-
Safronova, 2005	353	-	-
Martenson, 1995	317	-0.069	339
This work, 2019	214	-0.16	248

$A_{exp} = 265$ MHz

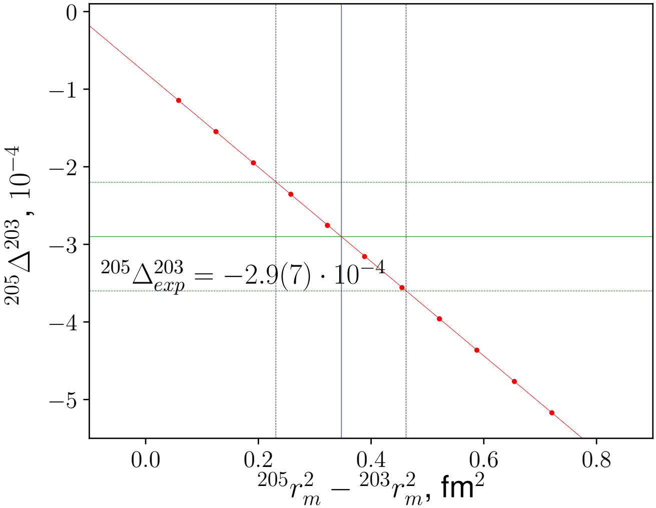
Calculation of hyperfine anomaly $6P_{1/2}$



Calculation of hyperfine anomaly $6P_{3/2}$



Calculation of hyperfine anomaly $7S_{1/2}$



Magnetic moment extraction

$A_1[a], A_2[b], A_2[a], A_1[b]$ – experimental HFS for electronic states a,b for isotopes 1,2.

μ_1 is known.

$\frac{A_1[a]}{A_2[b]} \frac{A_2[a]}{A_1[b]} = \frac{1+{}^1\Delta^2[a]}{1+{}^1\Delta^2[b]} = 1 + {}^1\theta^2[a, b]$ ${}^1\theta^2[a, b]$ – exp.

${}^1\Delta^2[b] = \frac{{}^1\theta^2[a,b]}{{}^1\Delta^2[a]/{}^1\Delta^2[b] - {}^1\theta^2[a,b] - 1}$ ${}^1\Delta^2[a]/{}^1\Delta^2[b]$ – theor.

$$\mu_2 = \mu_1 \cdot \frac{A_2[b]}{A_1[b]} \cdot \frac{I_2}{I_1} \cdot (1 + {}^1\Delta^2[b])$$

Magnetic moment extraction ^{193}Tl

$\mu_{\text{exp}}(^{205}\text{Tl}) = 1.63821461(12)$

$^{205}\theta^{193}[7\text{S}_{1/2}, 6\text{P}_{1/2}] = -0.013(7)$ (exp)

$\frac{\Delta(7\text{S}_{1/2})}{\Delta(6\text{P}_{1/2})} = 3.4$ (Theor.)

This work: $\mu(^{193}\text{Tl}) = 3.84(3)$ $\mu(^{191}\text{Tl}) = 3.79(2)$

Barzakh et al*: $\mu(^{193}\text{Tl}) = 3.82(3)$ $\mu(^{191}\text{Tl}) = 3.78(2)$

*A. Barzakh, L. K. Batist, D. Fedorov, V. Ivanov, K. Mezilev, P. Molkanov, F. Moroz, S. Y. Orlov, V. Panteleev, and Y. M. Volkov, Physical Review C 86, 014311 (2012).

Conclusion

- The calculation of the Bohr–Weisskopf correction and the magnetic anomaly can be made in the Gaussian basis ⇒ it is possible to perform calculations for molecules.
- To improve the description of nuclei:
    - Fermi charge distribution.
    - Saxon–Woods potential for a valence nucleon (magnetization distribution).
- To obtain the magnetic moments of short-lived nuclei, the ratio of anomalies for two electron states should be considered.
- In the long run, the anomaly can be used to test nuclear models.

Thank you for your attention!

- Point dipole:

$$\vec{A}(r) = \frac{\vec{\mu} \times \vec{r}}{r^3}$$

- Uniformly magnetized ball:

$$\vec{A}(r) = \frac{\mu}{R_M} \frac{r_<}{r_>^2} \sin\theta \begin{pmatrix} -\sin\varphi \\ \cos\varphi \\ 0 \end{pmatrix}$$