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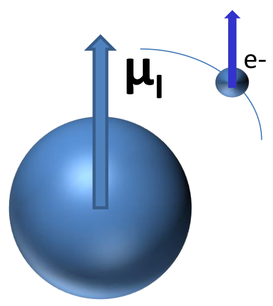
Nuclear magnetization distribution effect in molecules and atoms

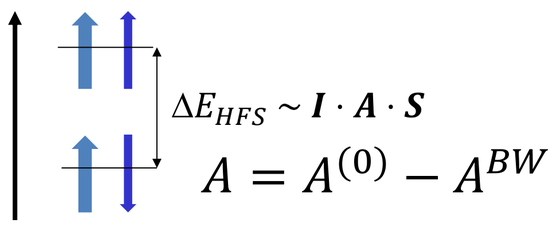
Leonid V. Skripnikov

Petersburg Nuclear Physics Institute named by B.P. Konstantinov of NRC «Kurchatov Institute»

INTRODUCTION & AIM

Hyperfine structure and the nuclear magnetization distribution effect in molecules and atoms





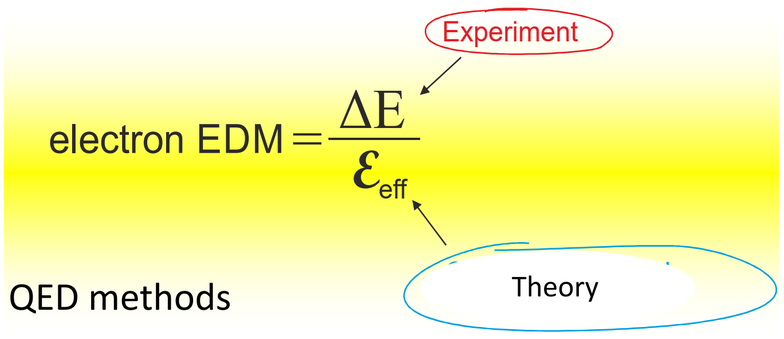
$\Delta E = \Delta E_0 - \Delta E_{BW}$

HFS within the point magnetic dipole approximation

Contribution from finite nuclear magnetization distribution: Bohr – Weisskopf effect (BW)

Why do we need HFS?

- ✓ Probe the accuracy of calculated atomic and molecular constants characterizing symmetry-violating effects in searches for New physics



- ✓ Probe of bound-state QED methods
- ✓ Study of the nuclear structure: valence nucleon configuration, nuclear many-body effects, etc.

METHOD

Hyperfine interaction in the point magnetic dipole approximation:

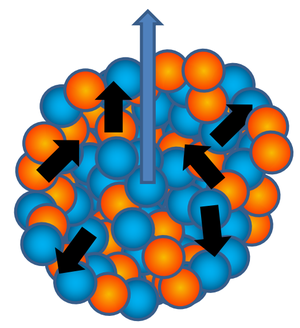
$$H_{HFI} = \boldsymbol{\mu} \cdot \frac{[\boldsymbol{r} \times \boldsymbol{\alpha}]}{\mathrm{r}^3} \quad \Rightarrow \quad A^{(0)} = \frac{\mu}{I\Omega} \left\langle \Psi_\Omega \left| \frac{[\boldsymbol{r} \times \boldsymbol{\alpha}]_z}{\mathrm{r}^3} \right| \Psi_\Omega \right\rangle$$

Hyperfine interaction with finite nuclear magnetization distribution:

$$H_{HFI} = \boldsymbol{\mu} \mathrm{F(r)} \cdot \frac{[\boldsymbol{r} \times \boldsymbol{\alpha}]}{\mathrm{r}^3} \quad \Rightarrow \quad A = A^{(0)} - A^{BW}$$

$$A^{(BW)} = \frac{\mu}{I\Omega} \left\langle \Psi_\Omega \left| \frac{[\boldsymbol{r} \times \boldsymbol{\alpha}]_z}{\mathrm{r}^3} (1 - \mathrm{F(r)}) \right| \Psi_\Omega \right\rangle$$

- ➢ **F(r) is the nuclear magnetization distribution function.**
- ➢ 1- F(r) is localized inside the nucleus



- ➢ **We do not know F(r) accurately, but this is not important!**

Factorization of the BW effect contribution to the hyperfine structure constant [1]:

$$A^{BW} = \frac{\mu}{I\Omega} (\mathcal{P}_s + \beta \mathcal{P}_p) B_s \qquad B_s = \frac{1}{2\mu} A_{BW}(\mathrm{H-like\ ion})$$

Pure electronic part

Universal nuclear-model-dependent parameter for a given heavy element

The BW effect A^{BW} can be factorized into purely electronic and nuclear-dependent parts B_s due to [1]:

1.) only $s_{1/2}$ and $p_{1/2}$ states contribute to the BW effect.

2.) all ns1/2-type functions are proportional to the **1**s1/2 H function within the nucleus; all np1/2-type functions are proportional to the **2**p1/2 H function within the nucleus.

3.) Special symmetry properties of the hyperfine interaction operator A^{BW}(2p1/2)~A^{BW}(1s1/2).

RESULTS & DISCUSSION

I. We combine electronic-structure coupled-cluster theory (CCSDT(Q)) with experiment to extract the Bs parameter (the BW effect for H-like ^{225}Ra) [1]

$$A^{BW} = A^{(0)}_{theory} - A(\mathrm{Ra^+})_{exp}$$

$$B_s(^{225}Ra) \text{ [F(r) for } ^{225}Ra]$$

TABLE II. BW contributions A^{BW}, $A^{BW,s}$, and $A^{BW,p}$ and the final values of the hyperfine structure constants (in MHz) for the ground and excited states of the $^{225}Ra^+$ cation. For the ground state, A^{BW} has been obtained as a difference between the theoretical value of the HFS constant calculated in the point magnetic dipole approximation and the experimental value taking into account QED and Breit effects.

	$7s\ ^2S_{1/2}$	$7p\ ^2P_{1/2}$	$7p\ ^2P_{3/2}$
$-A^{BW,s}$	1214	−5	3
$-A^{BW,p}$	1	80	0
$-A^{BW}$	1215	75	2
$A^{(0)}$ (see Table I)	−29012	−5526	−463
Breit+QED,[a] Ref. 3	66(23)		
Final	−27731	−5451	−461
Experiment[85–87]	−27731(13)	−5446.0(7)	−466.4(4.6)

[a]Extracted from Ref. 3: Breit: −93 MHz; QED: 159(23) MHz; Electron+Breit:−29113 MHz.

II. We predict the hyperfine structure constant for the RaF molecule without and with the finite nuclear magnetization distribution effect, using a universal Bs parameter and highly accurate CC methods [1]

TABLE III. Hyperfine structure constants $A_\parallel$ and $A_\perp$ (in MHz) for the ground $X^2\Sigma_{1/2}$ and excited $A^2\Pi_{1/2}$ states of the ^{225}RaF molecule induced by the ^{225}Ra nucleus.

Method	$X^2\Sigma_{1/2}$		$A^2\Pi_{1/2}$	
	$A_\parallel$	$A_\perp$	$A_\parallel$	$A_\perp$
$-A^{BW}_{\parallel/\perp}$	730	720[a]	44	26[a]
Final	−17049	−16403	−2852	−2204

III. Observation of the nuclear magnetization distribution in a molecule: the first highly accurate measurement by the CRIS collaboration [2] in a molecule containing an unstable nucleus

	Theory [1], no BW, MHz	Theory [1], with BW, MHz	Experiment 2025 [2] , MHz
$A_{\parallel}(^{225}\mathrm{RaF})$	-17**780**	-17**049**(170)	-17**064**(62)
$A_{perp}(^{225}\mathrm{RaF})$	-17**123**	-16**403**(164)	-16**324**(25)

CONCLUSION

- ✓ **Molecules can be used to probe the distribution of nuclear magnetization.**
- ✓ **The excellent agreement between theory and experiment validates the molecular parameter values characterizing T,P-odd violation effects (E_{eff}, W_S, $W_{T,P}$, W_A), which will be used in a future RaF experiment to probe New physics beyond the Standard model.**

REFERENCES

[1] L.V. Skripnikov, J. Chem. Phys. **153**, 114114 (2020)

[2] S.G. Wilkins et al, Science, **390**, 386 (2025)