Relativistic corrections to the hyperfine structure of hydrogen molecular ions

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Rovibrational spectroscopy of hydrogen molecular ions

- Sensitivity to fundamental constants

$$\nu = cR_\infty \left[\varepsilon_{nr}(\mu_{ne}) + \alpha^2 F_{QED}(\alpha) + \sum_n A_n^{fs} (r_n / a_0)^2 \right]$$

Schrödinger — Relativistic and QED corrections — Nuclear finite size correction

$$\nu_{vibr} \propto R_\infty \sqrt{m_e / m_r} \qquad \nu_{rot} \propto R_\infty m_e / m_r$$

H_2^+ $R_\infty, r_p, m_e / m_p$

HD^+ $R_\infty, r_p^2 + r_d^2, m_e / m_r^{(pd)}$

- Experiments may soon reach a few **10^{-12}** using Doppler-free schemes
- Theoretical accuracy of spin-averaged vibrational transitions = **7.5 10^{-12}**
- However, the theory/exp comparison is limited by the hfs!

LKB

Status of HD^+ hyperfine structure theory

Spin-orbit — Nuclear spin-rotation — Spin-spin Fermi contact interaction

$$H_{\mathrm{eff}} = E_1(\mathbf{L}\cdot\mathbf{s}_e) + E_2(\mathbf{L}\cdot\mathbf{I}_p) + E_3(\mathbf{L}\cdot\mathbf{I}_d) + E_4(\mathbf{I}_p\cdot\mathbf{s}_e) + E_5(\mathbf{I}_d\cdot\mathbf{s}_e)$$

$$+ E_6\left\{2\mathbf{L}^2(\mathbf{I}_p\cdot\mathbf{s}_e) - 3[(\mathbf{L}\cdot\mathbf{I}_p)(\mathbf{L}\cdot\mathbf{s}_e) + (\mathbf{L}\cdot\mathbf{s}_e)(\mathbf{L}\cdot\mathbf{I}_p)]\right\}$$

$$+ E_7\left\{2\mathbf{L}^2(\mathbf{I}_d\cdot\mathbf{s}_e) - 3[(\mathbf{L}\cdot\mathbf{I}_d)(\mathbf{L}\cdot\mathbf{s}_e) + (\mathbf{L}\cdot\mathbf{s}_e)(\mathbf{L}\cdot\mathbf{I}_d)]\right\}$$

$$+ E_8\left\{2\mathbf{L}^2(\mathbf{I}_p\cdot\mathbf{I}_d) - 3[(\mathbf{L}\cdot\mathbf{I}_p)(\mathbf{L}\cdot\mathbf{I}_d) + (\mathbf{L}\cdot\mathbf{I}_d)(\mathbf{L}\cdot\mathbf{I}_p)]\right\}$$

Spin-spin tensor interactions

$$+ E_9\left\{\mathbf{L}^2\mathbf{I}_d^2 - \frac{3}{2}(\mathbf{L}\cdot\mathbf{I}_d) - 3(\mathbf{L}\cdot\mathbf{I}_d)^2\right\}$$

Deuteron Quadrupole moment

- ✓ Calculations at the Breit-Pauli level (~α^2 relative accuracy)

  D. Bakalov, V.I. Korobov, S. Schiller, PRL **97**, 043001 (2006)

(L=1,v=0)
Unit: MHz

E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8	E_9
31.9846	-3.134[-02]	-4.809|-03]	924.629	142.146	8.6111	1.3218	-3.057[-03]	5.666[-03]

2 (E_1) — 1 (E_4, E_5) — 3 (E_6, E_7)

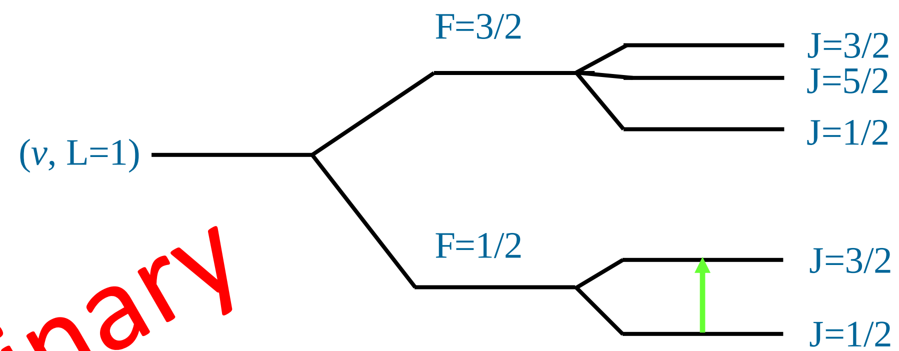
- ✓ Higher-order corrections to E_4, E_5

  V.I. Korobov, J.C.J. Koelemeij, L. Hilico, J.-Ph. Karr, PRL **116**, 043001 (2016) (H_2^+)

- ➢ Next step: $(Z\alpha)^2$ relativistic correction to E_1 ; then E_6, E_7

Comparison with experiments: H_2^+

$$H_{eff} = b_F(\mathbf{I}.\mathbf{s_e}) + c_e(\mathbf{L}.\mathbf{s_e}) + c_I(\mathbf{L}.\mathbf{I}) + \frac{d_1}{(2L-1)(2L+3)}\left\{\frac{2}{3}\mathbf{L}^2(\mathbf{I}.\mathbf{s_e}) - [(\mathbf{L}.\mathbf{I})(\mathbf{L}.\mathbf{s_e}) + (\mathbf{L}.\mathbf{s_e})(\mathbf{L}.\mathbf{I})]\right\}$$
$$+ \frac{d_2}{(2L-1)(2L+3)}\left\{\frac{1}{3}\mathbf{L}^2\mathbf{I}^2 - \frac{1}{2}(\mathbf{L}.\mathbf{I}) - (\mathbf{L}.\mathbf{I})^2\right\}$$



Preliminary

RF spectroscopy experiments

S.C. Menasian, PhD Thesis (1973)

ro-vibrational level	Δc_e (kHz)
$(L=1, v=4)$	0.81
$(L=1, v=5)$	0.74
$(L=1, v=6)$	0.67

[1]	This work (present)	Experiment
15.371049	15.371447	15.371407(2)
14.381189	14.381553	14.381513(2)
13.413169	13.413498	13.413460(2)

Unit : MHz

[1] V.I. Korobov, J.C.J. Koelemeij, L. Hilico, J.-Ph. Karr, PRL **116**, 043001 (2016)

- Numerical calculations of the correction to ***tensor interactions*** are in progress.