The hyperfine structure of the hydrogen molecular ion

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Outline

- Hyperfine structure (hfs) in H *vs* H_2^+
- Measurements of hfs in H_2^+
- Calculations of hfs
- Deuterium molecular ion D_2^+
- Future

Progress in H_2^+ precision work

- 3-body Schrödinger equation
- Born-Oppenheimer fixed (clamped) nuclei
- Adiabatic
- Nonadiabatic
- Full variational (Yan, Drake, Korobov, …)
- Relativistic: Dirac. Breit-Pauli $O(\alpha^2)$ Ry
- Radiative $O(\alpha^3)$ Ry
- And higher

Hyperfine interaction

- Studied over many decades
- Original motivation astrophysical
- Similar to hydrogen molecule , however…
- H_2 is diamagnetic, while H_2^+ is paramagnetic.

H (atom)

$1\ ^2S_{1/2} \quad I = \frac{1}{2};\ F = 1 \rightarrow 0$

Experiment

$\Delta\nu_{hfs} = 1420.4057517667(9)$

Hellwig et al. 1970 CfA

Theory

Let's see…

H (atom)

$$\Delta\nu_{hfs} = 1420.4057517667(9)$$

Main effect: $\mathbf{I}\cdot\mathbf{S}$

Electron motion→current density→mag. field

Proton has magnetic moment $\vec{\mu} = \mu_N g_N \mathbf{I}$

$$\Delta\nu_{\text{Fermi}} = \tfrac{8}{3}\pi g_e \mu_0 g_N \mu_N \langle\delta(\mathbf{r})\rangle$$

=1422.808 MHz

H (atom)

$\Delta\nu_{hfs} = 1420.4057517667(9)$

Other corrections

Finite mass of proton: introduces a factor

$$\left(\frac{1}{1+\frac{m_e}{M_p}}\right)^3$$

Inclusion gives 1420.486 MHz

Still more… with QED 1420.45199(14)

Best theory 1420.405(2) MHz

Experimental data

- Dehmelt group ca. 1960's, 3 kHz level. RF Paul trap. $v \geq 4$
- Carrington group, highly excited v states. Beam apparatus.
- Fu, Hessels, Lundeen 1992, 20-30 kHz. Rydberg hydrogen molecule, $v=1$
- Osterwalder, Wüest, Merkt, Jungen, 2004. Rydberg hydrogen molecule. 300 kHz. $v=1$

hfs Hamiltonian

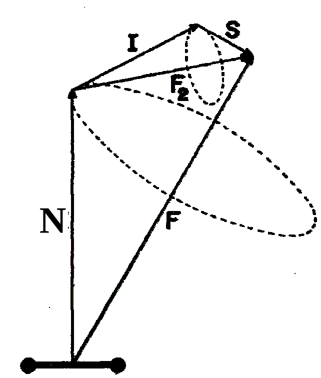
H_2 $\quad {}^1\Sigma_g^+ \; v=0, N=1, \; F=|\mathbf{I}+\mathbf{N}|, S=0$

H_2^+

Recall, presence of electron spin (paramagnetic)

${}^2\Sigma_g^+ \; v=0, N=1, \; F_2, F, \; S=\frac{1}{2}$

$$H_{\rm hfs} = (b_{1F} - \tfrac{1}{3}c)\mathbf{I}\cdot\mathbf{S} + cI_zS_z + d\mathbf{S}\cdot\mathbf{N} + f\mathbf{I}\cdot\mathbf{N}$$



Mass effect in H_2^+

- Studied adiabatic approximation.
- Fermi contact, for example, results come out about 600 kHz larger than fit to expt.
- Include action of nuclear kinetic energy on electronic wave function ∇_R^2
- "Nonadiabatic effects"

hfs Hamiltonian

$$H_{\rm hfs} = (b_{1F} - \tfrac{1}{3}c)\mathbf{I}\cdot\mathbf{S} + cI_zS_z + d\mathbf{S}\cdot\mathbf{N} + f\mathbf{I}\cdot\mathbf{N}$$

Korobov, Hilico, Karr (06)

$$\begin{aligned} H_{\rm eff} = {} & b_F(\mathbf{I}\cdot\mathbf{s}_e) + c_e(\mathbf{L}\cdot\mathbf{s}_e) + c_I(\mathbf{L}\cdot\mathbf{I}) \\ & + \frac{d_1}{(2L-1)(2L+3)}\left(\frac{2}{3}\mathbf{L}^2(\mathbf{I}\cdot\mathbf{s}_e) - [(\mathbf{L}\cdot\mathbf{I})(\mathbf{L}\cdot\mathbf{s}_e) \right. \\ & \left. + (\mathbf{L}\cdot\mathbf{s}_e)(\mathbf{L}\cdot\mathbf{I})]\right) + \frac{d_2}{(2L-1)(2L+3)}\left(\frac{1}{3}\mathbf{L}^2\mathbf{I}^2 \right. \\ & \left. - \frac{1}{2}(\mathbf{L}\cdot\mathbf{I}) - (\mathbf{L}\cdot\mathbf{I})^2\right). \end{aligned}$$

Frequencies

- Korobov *et al*. to 1-2 kHz with expt. (For v=0, N=1, Korobov *et al*. agree with our previous to within 8 kHz, for Fermi 2 kHz.).
- Remaining discrepancies, certain transitions, about 80 kHz, spin-flip.

  $O(\alpha^4 Ry \frac{m_e}{M_p})$

Deuteron static electric quadrupole moment

Nuclear physics experiment

$$^{208}\mathrm{Pb} + d \rightarrow {}^{208}\mathrm{Pb} + d$$

$Q = 0.282 \pm 0.019 \times 10^{-26}\mathrm{cm}^2$

Kammeraad,Knutson 85

Molecular physics

- Measurements possible
- Enters hfs through *eqQ* and couples nuclear spin and molecular rotation
- Diamagnetic system “purest”. E.g. Code and Ramsey (1974) measured to 25 **Hz**.

Calculations many electrons

For D_2, calculations of

$$q \sim \langle \frac{1}{R^3} - \sum_i \frac{3\cos^2\theta_i - 1}{r_i^3} \rangle$$

sum over all electrons

Reid,Vaida 1974; Bishop,Cheung 1978

$Q = 0.2860 \pm 0.0015 \times 10^{-26}\mathrm{cm}^2$

Another molecule: LiD (need q)

$Q = 0.29 \times 10^{-26}\mathrm{cm}^2$

Freeman et al. 1975; Kirby Docken,Freeman 1974

Ions?

- Why not HD^+
- Calculations by Bakalov, Korobov, and Schiller 2006, 10 kHz effect.
- Why not D_2^+?

D_2^+

- One measurement of ground state hfs (Cruse, Jungen, Merkt, 08) using Rydberg D_2
- Hfs to 300 kHz.
- Present includes nonadiabatic.

Level position (F,G)	Present	CJM`08
(5/2,3/2)	80.597	80.3(3)
(3/2,3/2)	70.319	70.9(3)
(1/2,3/2)	47.878	47.2(4)
(1/2,1/2)	–136.436	–137.2(4)
(3/2,1/2)	–146.94	–146.3(4)

Anti-H2+

Dehmelt, 1988

antiproton plasma in a r.f. trap. Currently most promising for atomic antimatter physics is the antiparticle of the molecular hydrogen ion H_2^+, with rich r.f. and infrared spectra. In a Paul r.f. trap, loaded with a plasma of many LCR-cooled positrons and a few antiprotons, synthesis and confinement of it and possibly even a singly charged polymolecular antihydrogen cluster seem feasible today. The forbidden microwave and infrared spectra of an individual diatomic molecular ion of antihydrogen might then be measured to a revolutionary resolution, and be compared to those of the normal molecular ion.

Anti-H2+

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Economic Synthesis and Precision Spectroscopy of Anti-Molecular Hydrogen Ions in Paul Trap

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Abstract

Estimates of operating parameters of a Paul trap suitable for synthesis and spectroscopy of anti-molecular hydrogen ions are presented. The trap may employ a 2-frequency trapping voltage. Transportable cryogenic Paul traps for the long-time storage of positrons and antiprotons may make such experiments possible in an average university lab in the not too distant future.

It may be possible [1] to produce simple charged anti-matter molecules from positrons confined in a Paul rf quad-rupole trap and antiprotons contained simultaneously [2] by the space charge of the positrons. The trap with the

Molecular ions

- Other systems: H_2D^+ and D_2H^+
- Asvany, Schlemmer (2008, Köln): 20 kHz. Expt
- Theory about 50 MHz away.
- Future sympathetic cooling
- If you find two nuclei too few,

Conclusions

- Theoretical work on H_2^+ in good shape thanks to Korobov and collaborators
- More experimental data needed
- D_2^+ still largely unexplored experimentally, though paramagnetism limits precision
- What about anti-matter molecular ions?