The H_2 molecule; test of QED and varying constants

Wim Ubachs
Department of Physics and Astronomy, LaserLaB, VU University, De Boelelaan 1081, 1081 HV Amsterdam, Netherlands
Author e-mail address: w.m.g.ubachs@vu.nl

Abstract: Calculations of QED effects in molecules are tested by precision laser spectroscopy in H_2, HD and D_2. The same hydrogen molecule is used to probe variation of the proton-electron mass ratio on a cosmological time scale.
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1. Introduction: QED phenomena

Quantum electrodynamics (QED) has been hailed as the most successful theory in physics as its predictions are in remarkable agreement with a variety of extremely precise experiments. Recently, the problem of QED calculations (also including high-order relativistic corrections) in the smallest neutral molecule H_2, the benchmark system of molecular physics, has been addressed by Pachucki and co-workers, and highly accurate calculations can now be performed [1]. Those can be tested in a number of experiments. The hydrogen molecule, as the most abundant molecule in the Universe is also a probe to search for variation of the proton-electron mass ratio on a cosmological time scale.

2. Measurement of the dissociation limit of hydrogen

Experimentally the ionization limit of the hydrogen isotopomers was determined in a combination of three experiments: (1) the energy separation between $X^1\Sigma_g^+$, v=0, J=1 and $EF^1\Sigma_g^+$, v=0, J=1 was determined via Doppler-free two-photon excitation using a narrowband pulsed UV-laser [2]; (2) the separation between $EF^1\Sigma_g^+$, v=0, J=1 and $54p1_1(0)$ measured in one photon spectroscopy [3]; (3) the extrapolation of millimeter wave spectroscopy on the Rydberg series to determine the ionization limit [4]. This leads to values of the dissociation limit presented in Table 1. These measurements test the QED contribution to the binding energies of 0.1964(9) cm^{-1} (for the case of H_2).

Table 1: Experimental and theoretical values for the dissociation limits of the hydrogen isotopomers. All values in cm^{-1}.

	Experiment	Theory [1]
$E_{diss}(H_2)$	36118.0696(4) [3]	36118.0695(10)
$E_{diss}(HD)$	36405.7837(4) [5]	36405.7828(10)
$E_{diss}(D_2)$	36748.3629(7) [6]	36748.3633(9)

3. QED test on rotational quantum states in H_2

In an independent experiment Doppler-free two-photon laser excitation in the $EF^1\Sigma_g^+$ - $X^1\Sigma_g^+$ system was performed for a progression of rotational states in H_2. High rotational quantum states up to J=16 were prepared by a photochemical process involving photolysis of HBr molecules, and a subsequent reaction H + HBr $\rightarrow$ Br + H_2(J). The information from the accurately calibrated lines was transferred to binding energies of the H_2, v=0, J states; from the resulting values the (theoretical) non-QED values were subtracted in order to make a comparison of QED-effects in the rotational sequence in H_2 [7]. The comparison is shown in Fig. 1.

4. QED test on the fundamental ground tone splitting

The fundamental ground tone of the H_2 molecule (for the rotationless case) was recently measured by a combination of two two-photon experiments, resulting in an accurate value for the splitting energy. Since for the case of rotationless quantum states fortuitous cancellations occur in the non-adiabatic and QED calculations these measurements provide a stringent test of those QED calculations [8].

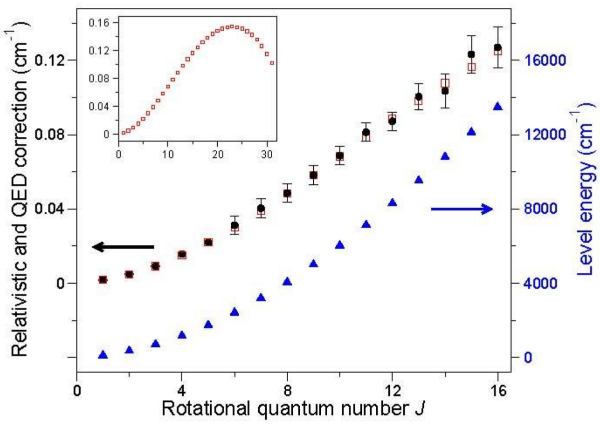

Fig. 1: Rotational level energies of H_2, v=0, J states (triangles and righthand scale). Experimentally determined (black symbols) and theoretically calculated values for the QED and high-order relativistic effects (lefthand scale, corrected for the shift of the J=0 level: 0.7283 cm^{-1}).

5. Variation of the proton-electron mass ratio from quasar spectra

The H_2 molecule is the most abundant molecule in the Universe and its electronic absorption spectrum can be observed with ground-based telescopes for redshifts z>2. The best of those observations typically constrain the proton-electron mass ratio to $\Delta\mu/\mu < 1 \times 10^{-5}$ for look-back times of some 12 billion years [9]. Recently we have performed an observation of hydrogen at redshift z = 4.2, which should provide a limit on a varying constant in earlier stages of the universe.

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