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Quadrupole transitions of the hydrogen molecular ion HD^+

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HD^+ hydrogen molecular ion is of metrological interest due to possibility of precise theoretical evaluation of its spectrum and of external-field-induced shifts. In present work, the rates of laser-induced electric quadrupole transitions are calculated for a wide range of rovibrational transitions in particular for L0-L'2, L1-L'3, L2-L'4 (v=(0-10)-v'=(0-3)). Results are presented with six significant digits.

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1. Introduction

Molecular hydrogen ions are three-body systems that allow for precise theoretical evaluation of their spectrum and external field effects [1, 2]. Properly selected transitions exhibit weak sensitivity to external fields. This feature makes them excellent candidates for frequency standards with potential uncertainties at the 10^{-17} fractional level [3, 4]. Current and future results from precision spectroscopy of molecular hydrogen ions, combined with the theoretical prediction of transition frequencies, also allow determining the fundamental constants of atomic physics, such as the proton-to-electron mass ratio and/or Rydberg constant [5, 6, 7, 8]. In homonuclear molecules H_2^+ the electric quadrupole transitions has been explored recently [9, 10]. So far only the dipole transition for HD$^+$ ion have been considered in the literature [11, 12]. Here, we present a complete consideration of the electric quadrupole transitions in HD$^+$, namely, the rates for transitions between states with vibrational quantum number up to $v=10$ are calculated. Thus the main motivation of this work is to provide the experimentalists with new data for the precision spectroscopy of the transitions, which are not accessible by the conventional dipole E1 spectroscopy due to the selection rules.

In what follows atomic units are used: $e^2/4\pi\varepsilon_0 = \hbar = m_e = 1$.

2. Interaction with laser-induced electromagnetic field

In the center-of-mass frame, the nonrelativistic Hamiltonian of HD$^+$ is

$$H^{\mathrm{NR}} = \frac{\mathbf{P}_1^2}{2m_p} + \frac{\mathbf{P}_2^2}{2m_d} + \frac{\mathbf{P}_e^2}{2} - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{R}, \tag{2.1}$$

here $\mathbf{R}_{1,2}$, $\mathbf{R}_e$ and $\mathbf{P}_{1,2}$, $\mathbf{P}_e$ are the position vectors relative to the center of mass and momentum operators of the proton, deuteron and the electron, respectively; $\mathbf{r}_1 = \mathbf{R}_e - \mathbf{R}_1$, $\mathbf{r}_2 = \mathbf{R}_e - \mathbf{R}_2$, $\mathbf{R} = \mathbf{R}_2 - \mathbf{R}_1$, and m_p and m_d are the masses of the proton and deuteron respectively.

The interaction Hamiltonian of a system of particles with external electromagnetic field is taken in a form [13]:

$$H_{\mathrm{int}} = -\sum_\alpha \frac{Z_\alpha}{m_\alpha} \mathbf{P}_\alpha \cdot \mathbf{A}(\mathbf{r}_\alpha, t), \tag{2.2}$$

here Z_α is the charge of particle α, $\alpha = p, d, e^-$. For a plane wave with general polarization the electromagnetic vector potential is

$$\mathbf{A}(\mathbf{r},t) = \mathbf{A}_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + \mathbf{A}_0^* e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)}, \tag{2.3}$$

where $\mathbf{A}_0$ is a complex vector satisfying $\mathbf{A}_0 \cdot \mathbf{k} = 0$.

3. $E2$ transition

In the long-wavelength approximation, we expand the exponent $e^{\pm i(\mathbf{k}\cdot\mathbf{r}_\alpha)}$ in (2.2) and keep only the terms responsible for the electric quadrupole transitions:

$$H_{\mathrm{int}}^{(E2)} = -\frac{i}{2\omega} \sum_{ij} T_{ij}^{(2)}(t) Q_{ij}^{(2)} \tag{3.1}$$

Table 1: Einstein coefficients A_{if} for selected $E2$ transitions in HD$^+$ in the "no-spin" approximation. ($a[b] = a\times10^b$)

$v-v'$	$L0-L2$	$L1-L3$	$L2-L4$	$v-v'$	$L0-L2$	$L1-L3$	$L2-L4$
0 − 0	0.266940[−11]	0.435701[−10]	0.255392[−9]	6 − 0	0.109985[−14]	0.192045[−11]	0.586954[−11]
0 − 1	0.791658[−7]	0.111358[−6]	0.133021[−6]	6 − 1	0.811070[−10]	0.181600[−11]	0.116964[−10]
0 − 2	0.127731[−7]	0.198443[−7]	0.259890[−7]	6 − 2	0.295509[−8]	0.708346[−9]	0.130802[−9]
0 − 3	0.171828[−8]	0.296236[−8]	0.423923[−8]	6 − 3	0.405839[−7]	0.152499[−7]	0.734931[−8]
1 − 0	0.272068[−6]	0.139067[−6]	0.997554[−7]	7 − 0	0.625284[−12]	0.201607[−11]	0.382213[−11]
1 − 1	0.266897[−11]	0.435159[−10]	0.254664[−9]	7 − 1	0.194906[−11]	0.481496[−11]	0.220544[−10]
1 − 2	0.132521[−6]	0.185470[−6]	0.220277[−6]	7 − 2	0.343277[−9]	0.252956[−10]	0.974395[−11]
1 − 3	0.329693[−7]	0.507206[−7]	0.658087[−7]	7 − 3	0.679764[−8]	0.183041[−8]	0.464255[−9]
2 − 0	0.303869[−7]	0.132487[−7]	0.787383[−8]	8 − 0	0.805157[−12]	0.139022[−11]	0.215779[−11]
2 − 1	0.460505[−6]	0.235947[−6]	0.169543[−6]	8 − 1	0.116000[−11]	0.795083[−11]	0.176212[−10]
2 − 2	0.262880[−11]	0.428172[−10]	0.250197[−9]	8 − 2	0.229204[−10]	0.416268[−11]	0.435431[−10]
2 − 3	0.165166[−6]	0.229968[−6]	0.271503[−6]	8 − 3	0.103362[−8]	0.130764[−9]	0.514987[−12]
3 − 0	0.251273[−8]	0.825326[−9]	0.318860[−9]	9 − 0	0.636455[−12]	0.847346[−12]	0.117792[−11]
3 − 1	0.812577[−7]	0.359832[−7]	0.217973[−7]	9 − 1	0.301478[−11]	0.672682[−11]	0.114510[−10]
3 − 2	0.580358[−6]	0.298042[−6]	0.214510[−6]	9 − 2	0.155110[−12]	0.157690[−10]	0.439546[−10]
3 − 3	0.255290[−11]	0.415406[−10]	0.242387[−9]	9 − 3	0.119072[−9]	0.823735[−13]	0.559189[−10]
4 − 0	0.191120[−9]	0.323180[−10]	0.105875[−11]	10 − 0	0.435900[−12]	0.498525[−12]	0.644346[−12]
4 − 1	0.943559[−8]	0.325964[−8]	0.137441[−8]	10 − 1	0.297002[−11]	0.463701[−11]	0.691862[−11]
4 − 2	0.143895[−6]	0.646561[−7]	0.398618[−7]	10 − 2	0.487761[−11]	0.169802[−10]	0.327972[−10]
4 − 3	0.644725[−6]	0.331837[−6]	0.239192[−6]	10 − 3	0.373245[−11]	0.186296[−10]	0.761487[−10]
5 − 0	0.100321[−10]	0.202467[−13]	0.515660[−11]				
5 − 1	0.981315[−9]	0.202695[−9]	0.219196[−10]				
5 − 2	0.219660[−7]	0.793315[−8]	0.359596[−8]				
5 − 3	0.210720[−6]	0.959897[−7]	0.601524[−7]				

where

$$T^{(2)}_{ij} = \frac{1}{2}(k_iE_j(0,t)+k_jE_i(0,t)) \qquad \text{and} \qquad Q^{(2)}_{ij} = \frac{3}{2}\sum_\alpha Z_\alpha\left(r_{i\alpha}r_{j\alpha} - \frac{1}{3}(\mathbf{r}_\alpha)^2\delta_{ij}\right) \tag{3.2}$$

and $T^{(2)}_{ij}$ is the symmetric part of the tensor product of the electric field at the center of mass of the system [9].

The $E2$ transitions matrix element between initial $|i\rangle$ and final $|f\rangle$ states can be put in a form:

$$S_{if} = C^{L'M'}_{LM,1\mu}\frac{\langle v'L'\|Q^{(2)}\|vL\rangle}{\sqrt{2L'+1}}, \tag{3.3}$$

In our numerical calculations the rates of transitions are expressed in terms of the Einstein coefficients A_{fi},

$$A_{fi}/t_0^{-1} = \frac{\alpha^5}{15(2L+1)}\Big(\big(E^{NR}_{v'L'} - E^{NR}_{vL}\big)/\mathscr{E}_0\Big)^5 \cdot \Big(\langle v'L'\|Q^{(2)}\|vL\rangle/\big(ea_0^2\big)\Big)^2 \tag{3.4}$$

where a_0, $t_0 = a_0/\alpha c$, and $\mathscr{E}_0 = 2\text{Ry}$ are the atomic units of length, time, and energy.

4. Results and conclusion

The numerical calculations were performed with the variational approach based on the exponential expansion with randomly chosen exponents [14]. Typical basis set were $N = 3000 - 4000$ that garantee precision for transitions rates at the level of 6 sigficiant digits. Numerical results for spontaneous transition rates ignoring spin structure are presented in Table 1 in terms of the Einstein coefficients in s^{-1} units.

In conclusion, the matrix elements of the electric quadruple transition moment have been calculated for a wide range in particular for L0-L'2, L1-L'3, L2-L'4 (v=(0-10)-v'=(0-3)). These transitions largely covers possible experimental needs. The obtained results are of importance for future experiments. The calculated amplitudes may be used to estimate the laser intensity necessary to achieve a desired transition rate.

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References

[1] V. I. Korobov, J.C.J. Koelemeij, L. Hilico, and J.-Ph. Karr, Phys. Rev. Lett. **116**, 053003 (2016).

[2] D. Bakalov, V.I. Korobov, and S. Schiller, Phys. B: At. Mol. Opt. Phys. **44**, 025003 (2011).

[3] J.Ph. Karr, S. Patra, J.C.J. Koelemeij, J. Heinrich, N. Sillitoe, A. Douillet, and L. Hilico, J. Phys.: Conf. Ser. **723**, 012048 (2016).

[4] S. Schiller, D. Bakalov, and V.I. Korobov, Phys. Rev. Lett. **113**, 023004 (2014).

[5] J.C.J. Koelemeij, B. Roth,A. Wicht, I. Ernsting, and S. Schiller, Phys. Rev. Lett. **98**, 173002 (2007).

[6] J. Biesheuvel, J.-Ph. Karr, L. Hilico, K.S.E. Eikema, W. Ubachs, and J.C.J. Koelemeij, Nat. Commun. **7**, 10385 (2016).

[7] S. Alighanbari, M.G. Hansen, V.I. Korobov, and S. Schiller, Nat. Phys. Nature Physics **14**, 555 (2018).

[8] J.Ph. Karr, L. Hilico, J.C.J. Koelemeij, V.I. Korobov, Phys. Rev A **94**, 050501 (2016).

[9] V.I. Korobov, P. Danev, D. Bakalov, and S. Schiller, Phys. Rev A **97**, 032505 (2018).

[10] J.-Ph. Karr, J. Mol. Spectrosc. **300**, 37 (2014).

[11] H.O. Pilón and D. Baye, Phys. Rev A **88**, 032502 (2013).

[12] Q.L. Tian, L.Y. Tang, Z.X. Zhong, Z.C. Yan, and T.Y. Shi, J. Chem. Phys. **137**, 024311 (2012).

[13] C. Cohen-Tannoudji, B. Diu, and F. Laloe, Quantum Mechanics, Wiley-Interscience, New York, 2006.

[14] V.I. Korobov, D. Bakalov, and H.J. Monkhorst, Phys. Rev. A **59**, R919(R) (1999).