Bogoliubov laboratory of theoretical physics (JINR)

Kazakh National University

SPECTROSCOPY OF MOLECULAR HYDROGEN IONS

BEKBAEV A.K., AZNABAYEV D.T. AND KOROBOV V.I.

FFK-2017

19 MAY 2017, Warsaw, Republic of Poland

Relativistic corrections to the dipole polarizability of hydrogen molecular ions

INVESTIGATED OBJECTS

$$H_2^+ \quad HD^+ \quad D_2^+$$

OUTLINE

- Nonrelativistic dipole polarizability
- Relativistic corrections to the dipole polarizability
- Results

Nonrelativistic dipole polarizability

Nonrelativistic Schrödinger equation

$$(H_0 - E_0)\psi_0 = 0$$

$$H_0 = \frac{\mathbf{P}_1^2}{2M_1} + \frac{\mathbf{P}_2^2}{2M_2} - \frac{\mathbf{p}_e^2}{2m_e} + \frac{Z_1 Z_2}{R} - \frac{Z_1}{r_1} - \frac{Z_2}{r_2}$$

For states

$$J = 0 - 5 \qquad \nu = 0 - 10$$

The electric dipole

$$V_p = -\boldsymbol{\varepsilon} \cdot \mathbf{d}$$

$$\mathbf{d} = e[Z(\mathbf{R}_1 + \mathbf{R}_2) - \mathbf{r}]$$

The change of energy due to polarizability of molecular ions is expressed by

$$E_p^{(2)} = \left\langle \Psi_0 \mid V_p (E_0 - H_0)^{-1} V_p \mid \Psi_0 \right\rangle$$

$$= \varepsilon^i \varepsilon^j \left\langle \Psi_0 \mid d^i (E_0 - H_0)^{-1} d^j \mid \Psi_0 \right\rangle$$

$$= -\frac{1}{2} \alpha_d^{ij} \varepsilon^i \varepsilon^j$$

$$\alpha_d^{ij} = -2 \left\langle \Psi_0 \mid d^i (E_0 - H_0)^{-1} d^j \mid \Psi_0 \right\rangle$$

The polarizability tensor operator on a subspace of fixed total orbital angular momentum J expressed by:

$$\alpha_d^{ij} = \alpha_s + \alpha_t \left[J^i J^j + J^j J^i - \frac{2}{3} \mathbf{J}^2 \right]$$

$$\alpha_s = \frac{1}{3}[a_+ + a_0 + a_-]$$

$$\alpha_t = -\frac{a_+}{2(J+1)(2J+3)} + \frac{a_0}{2J(J+1)} - \frac{a_-}{2J(2J-1)}$$

S. Schiller, D. Bakalov, A.K. Bekbaev, V.I. Korobov PHYSICAL REVIEW A **89**, 052521 (2014)

The static dipole polarizability

$$a_{+} = \frac{2}{2J+1} \sum_{n} \frac{\langle 0\, J \,\|\, \mathbf{d} \,\|\, n\ (J+1) \rangle \langle n (J+1) \,\|\, \mathbf{d} \,\|\, 0\, J \rangle}{E_0 - E_n}$$

$$a_{0} = -\frac{2}{2J+1} \sum_{n} \frac{\langle 0\, J \,\|\, \mathbf{d} \,\|\, n\ \ J \rangle \langle n\, J \,\|\, \mathbf{d} \,\|\, 0\, J \rangle}{E_0 - E_n}$$

$$a_{-} = \frac{2}{2J+1} \sum_{n} \frac{\langle 0\, J \,\|\, \mathbf{d} \,\|\, n\ (J-1) \rangle \langle n (J-1) \,\|\, \mathbf{d} \,\|\, 0\, J \rangle}{E_0 - E_n}$$

Relativistic corrections to the dipole polarizability

$$\alpha_d = \alpha_d^{(nonrel)} + (1/c)^2 \alpha_B$$

Relativistic correction α_B

$$\alpha_B = 2\langle \Psi_B | \mathbf{d} | \Psi_1 \rangle + \langle \Psi_1 | H_B - \langle H_B \rangle | \Psi_1 \rangle$$

$$= 2\left\langle \Psi_0 | H_B Q (E_0 - H_0)^{-1} Q \mathbf{d} | (E_0 - H_0)^{-1} \mathbf{d} \Psi_0 \right\rangle$$

$$+ \left\langle \Psi_0 | \mathbf{d} (E_0 - H_0)^{-1} (H_B - \langle H_B \rangle)(E_0 - H_0)^{-1} \mathbf{d} | \Psi_0 \right\rangle$$

The Hamiltonian of the Breit-Pauli interaction for the three-body system

$$H_B = -\frac{\mathbf{p}_e^4}{8m_e^3} + \frac{4\pi}{8m_e^2}[Z_1\delta(\mathbf{r}_1) + Z_2\delta(\mathbf{r}_2)]$$

$$- \frac{\mathbf{P}_1^4}{8M_1^3} - \frac{\mathbf{P}_2^4}{8M_2^3} + \frac{Z_1}{2m_eM_1}\left(\frac{\mathbf{p}_e\mathbf{P}_1}{r_1} + \frac{\mathbf{r}_1(\mathbf{r}_1\mathbf{p}_e)\mathbf{P}_1}{r_1^3}\right)$$

$$+ \frac{Z_2}{2m_eM_2}\left(\frac{\mathbf{p}_e\mathbf{P}_2}{r_2} + \frac{\mathbf{r}_2(\mathbf{r}_2\mathbf{p}_e)\mathbf{P}_2}{r_2^3}\right)$$

$$- \frac{Z_1Z_2}{2M_1M_2}\left(\frac{\mathbf{P}_1\mathbf{P}_2}{R} + \frac{\mathbf{R}(\mathbf{R}\mathbf{P}_1)\mathbf{P}_2}{R^3}\right)$$

Ψ_B is the relativistic correction to the nonrelativistic wave function Ψ_0

$$\Psi_B = Q(E_0 - H_0)^{-1} Q H_B \,|\, \Psi_0$$

RESULTS

Test of convergence of the numerical results

for H_2^+

N	E_{NR}	α_d	$(1/c)^2\alpha_{\mathrm{B}} \times 10^2$
2000	−0.59713 90631 23404 0757	3.16872 58022 7017	−1.52753848
3000	−0.59713 90631 23405 0374	3.16872 58026 7529	−1.52753844
4000	−0.59713 90631 23405 0730	3.16872 58026 7610	−1.52753841
5000	−0.59713 90631 23405 0747	3.16872 58026 7613	−1.52753839

S. Schiller, D. Bakalov, A.K. Bekbaev, V.I. Korobov PHYSICAL REVIEW A **89**, 052521 (2014)

Table 1. Polarizability of the H_2^+ molecular ion (in a.u.).

	$J=0$	$J=1$		$J=2$		$J=3$		$J=4$		$J=5$	
v	α_s	α_s	α_t	α_s	α_t	α_s	α_t	α_s	α_t	α_s	α_t
0	3.1685731	3.1781425	−0.8033502	3.1973545	−0.1931356	3.2262879	−0.0914433	3.2650990	−0.0544748	3.3139976	−0.0367128
1	3.8973934	3.9099178	−1.1441799	3.9350819	−0.2750942	3.9730164	−0.1302617	4.0239695	−0.0776116	4.0882763	−0.0523165
2	4.8213113	4.8378793	−1.6000406	4.8711902	−0.3847577	4.9214594	−0.1822335	4.9890778	−0.1086134	5.0745756	−0.0732459
3	6.0091177	6.0313112	−2.2129254	6.0759600	−0.5322677	6.1434165	−0.2521933	6.2342968	−0.1503867	6.3494400	−0.1014829
4	7.5602216	7.5903867	−3.0434518	7.6511105	−0.7322788	7.7429690	−0.3471380	7.8669387	−0.2071473	8.0243574	−0.1399094
5	9.6215210	9.6632217	−4.1811193	9.7472225	−1.0064538	9.8744707	−0.4774294	10.046534	−0.2851531	10.265571	−0.1928167
6	12.415730	12.474532	−5.7615463	12.593067	−1.3876642	12.772916	−0.6588237	13.016644	−0.3939470	13.327789	−0.2667717
7	16.290723	16.375602	−7.9965248	16.546853	−1.9273285	16.807161	−0.9160282	17.160827	−0.5485430	17.613818	−0.3721506
8	21.809221	21.935211	−11.228720	22.189694	−2.7088006	22.577348	−1.2892136	23.105612	−0.7734482	23.784904	−0.5259745
9	29.920158	30.113640	−16.036365	30.504982	−3.8730665	31.102663	−1.8465662	31.920118	−1.1104628	32.976304	−0.7574536
10	42.306376	42.616282	−23.446097	43.244214	−5.6711694	44.206322	−2.7100353	45.528226	−1.6347899	47.246401	−1.1195399

Table 2. Polarizability of the D_2^+ molecular ion (in a.u.).

	$J=0$	$J=1$		$J=2$		$J=3$		$J=4$		$J=5$	
v	α_s	α_s	α_t	α_s	α_t	α_s	α_t	α_s	α_t	α_s	α_t
0	3.0718385	3.0764328	−0.7579298	3.0856549	−0.1813369	3.0995081	−0.0852409	3.1180309	−0.0502995	3.1412711	−0.0335034
1	3.5528638	3.5584089	−0.9782491	3.5695458	−0.2340523	3.5862817	−0.1100231	3.6086695	−0.0649249	3.6367756	−0.0432467
2	4.1194070	4.1261334	−1.2485728	4.1396485	−0.2987404	4.1599666	−0.1404395	4.1871595	−0.0828801	4.2213195	−0.0552122
3	4.7910944	4.7993001	−1.5808434	4.8157922	−0.3782640	4.8405962	−0.1778400	4.8738102	−0.1049648	4.9155614	−0.0699351
4	5.5931121	5.6031855	−1.9903702	5.6234356	−0.4762945	5.6539046	−0.2239563	5.694727	−0.1322053	5.7460784	−0.0881031
5	6.5581008	6.5705539	−2.4969746	6.5955906	−0.5975866	6.6332784	−0.2810323	6.6838036	−0.1659331	6.7474075	−0.1106091
6	7.7288214	7.7443358	−3.1265993	7.7755297	−0.7483664	7.8225084	−0.3520083	7.8855305	−0.2078938	7.9649300	−0.1386246
7	9.1619614	9.1814571	−3.9136098	9.2206579	−0.9368846	9.2797220	−0.4407829	9.3590190	−0.2604042	9.4590076	−0.1737066
8	10.933664	10.958399	−4.9041347	11.008137	−1.1742218	11.083110	−0.5525959	11.183859	−0.3265811	11.311016	−0.2179523
9	13.147705	13.179427	−6.1610100	13.243217	−1.4754799	13.339457	−0.6945965	13.468847	−0.4106816	13.632332	−0.2742296
10	15.947847	15.989024	−7.7712522	16.071842	−1.8615859	16.196869	−0.8766962	16.365114	−0.5186156	16.577941	−0.3465270

Table 3. Polarizability of the HD^+ molecular ion (in a.u.).

	$J=0$	$J=1$		$J=2$		$J=3$		$J=4$		$J=5$	
v	α_s	α_s	α_t	α_s	α_t	α_s	α_t	α_s	α_t	α_s	α_t
0	395.27754	3.9899486	175.46989	4.0093758	13.826954	4.0386030	3.1905097	4.0777634	1.1013280	4.1270299	0.4731528
1	462.62017	4.7029195	205.18613	4.7267328	16.142249	4.7625805	3.7153046	4.8106388	1.2779012	4.8711642	0.5463772
2	540.64963	5.5690125	239.56394	5.5984707	18.814812	5.6429097	4.3189073	5.7025090	1.4799073	5.7776380	0.6295018
3	631.36149	6.6325616	279.45735	6.6693071	21.908555	6.7251653	5.0148197	6.7999232	1.7113981	6.8942638	0.7239099
4	737.27142	7.9543692	325.93821	8.0010358	25.503117	8.0716799	5.8197299	8.1666401	1.9772885	8.2866362	0.8312163
5	861.59725	9.6180552	380.37171	9.6782520	29.699534	9.7691277	6.7545125	9.8914502	2.2835914	10.046247	0.9533009
6	1008.5213	11.742867	444.52180	11.821446	34.627354	11.940196	7.8456173	12.100244	2.6377250	12.303109	1.0923369
7	1183.5771	14.499937	520.70922	14.604304	40.455664	14.762192	9.1270207	14.975296	3.0489087	15.245914	1.2507930
8	1394.2333	18.141977	612.04499	18.283320	47.409088	18.497399	10.643024	18.786825	3.5286700	19.155146	1.4313721
9	1650.8015	23.051744	722.79107	23.247524	55.792076	23.544383	12.452318	23.946515	4.0914633	24.459532	1.6367943
10	1967.8945	29.827372	858.93232	30.105532	66.026733	30.528154	14.633990	31.101840	4.7553467	31.835850	1.8692259

Thank you for your attention!