

Bethe logarithm for the hydrogen molecular ion H_2^+

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The mean excitation energy (the Bethe logarithm) is calculated for the lowest rotational (up to $L=4$) and vibrational (up to $v=4$) states of the hydrogen molecular ion H_2^+ . The calculations are based on a method of the direct integration over photon momenta. The estimated accuracy of obtained values is about 10^{-6} . The Araki-Sacher Q term is computed as well, which allows us to evaluate the leading order α^3 radiative correction to the rovibrational energies of the hydrogen molecular ion.

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Precise theoretical and experimental studies of the positive molecular ions of the hydrogen isotopes are of growing interest in recent years. The variational calculations of the nonrelativistic energy achieve precision up to 10^{-15} – 10^{-20} of a relative accuracy [1–5] and are improving constantly due to the increasing power of modern computers. These calculations are sensitive to the proton to electron mass ratio and, as expected, can lead to metrological application [1,6]. The next order corrections which are known as the leading order (α^2) relativistic corrections and originate from the Breit-Pauli Hamiltonian [7,8] have been obtained so far with much less accuracy. However, very accurate results for the case of helium excited states have been available already some time ago [9] and one may expect that the same accurate calculations should appear in the near future for the hydrogen molecular ions due to availability of high quality variational wave functions. The next step is the evaluation of the leading order radiative corrections because the calculation of the Bethe logarithm [7] (the key quantity in the radiative part) is a complicated numerical problem and a satisfactory solution has been obtained only in the last decade in Refs. [10–12] for the helium atom and in Ref. [13] for the one electron molecular systems. In this work we will concentrate on calculations of the leading α^3 order contribution due to radiative effects for the H_2^+ molecular ion.

The leading order [α^3 and $\alpha^3(m/M)$] spin independent contribution for a one electron molecular system can be expressed as follows [13–15]:

$$\begin{aligned} \delta^{(3)}E = \alpha^3 \sum_i \left[\frac{4Z_i}{3} \left(-\ln \alpha^2 - \beta(L, v) + \frac{19}{30} \right) \langle \delta(\mathbf{r}_i) \rangle \right. \\ \left. + \frac{2Z_i^2}{3M_i} \left(-\ln \alpha - 4\beta(L, v) + \frac{31}{3} \right) \langle \delta(\mathbf{r}_i) \rangle - \frac{14Z_i^2}{3M_i} Q(r_i) \right], \end{aligned} \quad (1)$$

where

$$\beta(L, v) = \frac{\langle \mathbf{J}(H_0 - E_0) \ln[(H_0 - E_0)/R_\infty] \mathbf{J} \rangle}{\langle [\mathbf{J}, [H_0, \mathbf{J}]]/2 \rangle} \quad (2)$$

is the Bethe logarithm, H_0 is the three-body nonrelativistic Hamiltonian, $\mathbf{J} = -\mathbf{p}_e + \sum_i Z_i \mathbf{p}_i / M_i$ is the electric current density operator of the system, and $Q(r)$ is the Q term introduced by Araki and Sucher [16],

$$Q(r) = \lim_{\rho \rightarrow 0} \left\langle \frac{\Theta(r - \rho)}{4\pi r^3} + (\ln \rho + \gamma_E) \delta(\mathbf{r}) \right\rangle.$$

Atomic units are adopted throughout this paper.

A numerical scheme for calculation of the Bethe logarithm has been presented in detail in [13]. The nonlinear parameters for the variational wave functions of intermediate states have been chosen equal to the ones used in the HD^+ calculations [13] and no further optimization is performed. For the case of nonzero angular momentum L of the initial state, intermediate states span over $L' = L, L \pm 1$ with the spatial parity $\pi = -(-1)^L$. For each L' we take a number of basis functions up to 5000.

Results of numerical calculations are shown in Table I. We estimate that the numerical precision for the Bethe logarithm for these states is about 10^{-6} . This accuracy is sufficient to provide the final precision for vibrational transition energies to be about 10^{-11} – 10^{-12} on the assumption that higher order corrections are included.

TABLE I. The Bethe logarithm for the lowest rotational, L , and vibrational, v , states of the hydrogen molecular ion H_2^+ .

	$v=0$	$v=1$	$v=2$	$v=3$	$v=4$
$L=0$	3.012246	3.012563	3.012696	3.012640	3.012394
$L=1$	3.012219	3.012531	3.012659	3.012598	3.012348
$L=2$	3.012161	3.012465	3.012583	3.012514	3.012256
$L=3$	3.012077	3.012366	3.012472	3.012390	3.012118
$L=4$	3.011967	3.012239	3.012327	3.012228	3.011941

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TABLE II. The Araki-Sacher Q term (first row) and expectation values of $\langle \delta^3(\mathbf{r}_N) \rangle$ (second row) for the lowest rotational, L , and vibrational, v , states of the hydrogen molecular ion H_2^+ .

	$v=0$	$v=1$	$v=2$	$v=3$	$v=4$
$L=0$	-0.13442623 0.206736477	-0.13128638 0.201310665	-0.12839258 0.196294590	-0.12573150 0.191662499	-0.12329169 0.187391848
$L=1$	-0.13426682 0.206491320	-0.13113693 0.201081174	-0.12825266 0.196079944	-0.12560075 0.191461983	-0.12316979 0.187204848
$L=2$	-0.13395046 0.206004543	-0.13084038 0.200625549	-0.12797507 0.195653845	-0.12534138 0.191063990	-0.12292803 0.186833735
$L=3$	-0.13395046 0.206004543	-0.13040135 0.199950377	-0.12756422 0.195022552	-0.12495762 0.190474472	-0.12257045 0.186284175
$L=4$	-0.13286841 0.204336990	-0.12982653 0.199065216	-0.12702649 0.194195147	-0.12445555 0.189702063	-0.12210286 0.185564385

Numerical calculation of the Q term is straightforward; results are presented in Table II. Using the data of the two tables in this work, the complete contribution of the α^3 order to the energies of the hydrogen molecular ion

can be obtained via Eq. (1) with a relative accuracy of 7–8 digits.

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