Hyperfine structure and relativistic corrections to ro-vibrational energies of HT$^+$ ions

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Abstract
We present systematic calculations of the leading order relativistic corrections for a wide range of rotational and vibrational states of the HT$^+$ molecular ion. Finite size effects are also taken into account. These are the first complete ab initio calculations, which may be used for precision spectroscopy of the ro-vibrational spectrum in HT$^+$. (Some figures may appear in colour only in the online journal)

1. Introduction
The molecular hydrogen ion isotopomers H$_2^+$ and HD$^+$ have been intensively studied over the last few years both theoretically [1–3] and experimentally [4, 5] with the aim to improve the determination of $m_e/m_p$, the proton-to-electron mass ratio, via ro-vibrational spectroscopy [6, 7].

The HT$^+$ molecular ion is a system which has been examined much less so far. On the other hand, it may be a good tool for exploration of properties of the heaviest hydrogen isotope—triton. The first systematic studies of this system were performed in the 1970s [8, 9]. More recent calculations were presented in [10] for the vibrational states with the total orbital momentum $L = 0$ and in [11] for a wider range of states, which also included states of the total orbital angular momentum $L = 0$ – 5 and vibrational quantum number $v = 0$ – 5. Results were obtained with a numerical fractional accuracy of less than $10^{-14}$. Hitherto all calculations$^3$ were performed in the nonrelativistic approximation.

In our present work we carry out extended calculations of the leading order relativistic corrections for HT$^+$ ro-vibrational states. It includes as well calculations of the hyperfine structure (HFS), which to our knowledge have never been published before for this isotopomer of the hydrogen molecular ion. The HFS may be of great importance for studies of the finite size properties of a triton, such as form factors, Zemach radius, etc.

2. Variational wave function and nonrelativistic energies
We adopt the following notation for the coordinate system of the three particles. Coordinates $\mathbf{R}_i$, $i = 1, 2, 3$ are position vectors of the triton, proton and electron, respectively, in the centre of mass frame. The vector $\mathbf{R} = \mathbf{R}_2 - \mathbf{R}_1$ is a relative position of the proton with respect to the triton, while $\mathbf{r}_1$ and $\mathbf{r}_2$ are the relative positions of the electron with respect to the triton and proton. Atomic units are used throughout: $m_e = \hbar = e = 1$.

The variational bound state wave functions were calculated by solving the three-body Schrödinger equation with Coulomb interaction using the variational approach based on the exponential expansion with randomly chosen exponents. This approach has been discussed in a variety of works [12–14]. Details and the strategy for choosing the variational nonlinear parameters and basis structure that have been used in the present work can be found in [15].

Briefly, the wave function for a state with a total orbital angular momentum $L$ and of a total spatial parity $\pi = (-1)^L$ is expanded as follows:

$$\Psi_{LM}^\pi(\mathbf{R}, \mathbf{r}_1) = \sum_{\hat{L}_1, \hat{L}_2 = L} \hat{Y}_{\hat{L}_1}^\pi(\mathbf{R}, \hat{r}_1) \hat{G}_{\hat{L}_1}^{\pi, L}(\mathbf{R}, r_1, r_2),$$

$$\hat{G}_{\hat{L}_1}^{\pi, L}(\mathbf{R}, r_1, r_2) = \sum_{n=1}^N \langle \mathbf{c}_n | \text{Re}[e^{-\alpha_n R - \beta_n r_1 - \gamma_n r_2}] \rangle + D_n \text{Im}[e^{-\alpha_n R - \beta_n r_1 - \gamma_n r_2}],$$

(1)
where the complex exponents, \( \alpha, \beta \) and \( \gamma \), are generated in a pseudorandom way.

When exponents \( \alpha_i, \beta_i \) and \( \gamma_i \) are real, the method reveals slow convergence for molecular type Coulomb systems. Thus, the use of complex exponents allows the oscillatory behaviour of the vibrational part of the wave function to be reproduced and the convergence to be improved [14, 15].

In the numerical calculations, the CODATA06 recommended values [16] have been used for the masses of a proton and triton, namely, \( M_p = 1836.15267247 m_e \) and \( M_t = 5496.9215269 m_e \).

The leading correction to the nonrelativistic energy is the \( \sigma^2 \) order relativistic correction determined by the Breit–Pauli Hamiltonian. It is derived in many different ways (see for example [17, 18]) for a system with a number of particles greater than 2. For a composite particle the finite size electromagnetic structure plays an important role, the interaction of such a particle with an electromagnetic field is discussed in [19]. In a more recent paper by Kinoshita and Nio [20] it is shown using nonrelativistic QED theory of how the electromagnetic structure of nuclei can be incorporated into the Breit–Pauli Hamiltonian in the correct way.

3. Fine and hyperfine splitting of the levels

The spin-dependent part of the Breit–Pauli Hamiltonian for a system of particles of spin 1/2 has the following form:

\[
H_{\text{HFS}} = -\frac{e^2}{c^2} \sum_{j \neq i} \frac{Z_J c_s^{(j)} [r_{ij} \times p_j] s_j}{2 m_j r_{ij}^3} \\
- \frac{e^2}{c^2} \sum_{i=1}^{N-1} \frac{Z_J c_s^{(i)} [r_{ij} \times p_i] s_i - c_{F_s}^{(i)} [r_{ij} \times p_i] s_j}{m_i m_j r_{ij}^3} \\
+ \sum_{i=1}^{N-1} \left\{ \frac{\mu_i \mu_j}{r_{ij}} - 3 \left( \frac{\mu_i \cdot r_{ij}}{r_{ij}} \right) \frac{\mu_j \cdot r_{ij}}{r_{ij}} \right\} - \frac{8\pi}{3} \mu_i \mu_j \delta(r_{ij}) \right) .
\]

(2)

Here \( \mu_i = (c_{F_s}^{(i)} Z_j/2m_i c) \sigma_i \) is an operator of magnetic moment, coefficients \( c_{F_s} \) and \( c_{S} \) are defined

\[
e_{F_s}^{(i)} = 1 + \kappa, \quad e_{S}^{(i)} = 1 + 2\kappa,
\]

where \( \kappa_i \) is an anomalous magnetic moment of a particle.

In actual calculations the following values of magnetic moments have been used:

\[
\mu_p = 2.792847337 \mu_N, \quad \mu_t = 2.978962448 \mu_N, \\
\mu_e = -1.001159652186 \mu_B.
\]

Anomalous magnetic moment \( \kappa_i \) for the triton may be expressed using our notations: \( \kappa_i = \mu_i (m_p/m_t) - 1 \).

The strongest coupling in the hyperfine interaction is due to the spin–spin electron–proton and electron–triton interactions. The spin–orbit interaction is much smaller. Thus we adopt the following coupling scheme:

\[
F = I_p + I_t, \quad S = F + s_t, \quad J = S + L.
\]

(3)

Operators \( F \) and \( S \) do not commute with the Hamiltonian, but still provide good approximate quantum numbers to describe HFS states of the system. Operator \( F \) is the total spin of nuclei, if \( F = 0 \) then spin–spin interaction is zero, however due to small coupling with other states final shifts are nonzero even for \( L = 0 \). The schematic diagram of the hyperfine states is shown in figure 1. By averaging the spatial variables of the Hamiltonian (2) one gets the effective Hamiltonian, which depends on the spin and orbital angular momentum variables (the spin–spin contact interaction between two nuclei is negligible):

\[
H_{\text{eff}} = E_1 (s_t \cdot I_p) + E_2 (s_t \cdot I_t) + E_3 (s_t \cdot L) \\
+ E_4 (I_p \cdot L) + E_5 (I_t \cdot L) + E_6 (2L(L+1)(s_t \cdot I_p) \\
- 3[(L \cdot s_p)(L \cdot I_p) + (L \cdot I_p)(L \cdot s_t)] + E_1(2L(L+1)(s_t \cdot I_t) \\
- 3[(L \cdot s_t)(L \cdot I_t) + (L \cdot L)(L \cdot s_t)]) + E_3(2L(L+1)(I_p \cdot I_t) \\
- 3[(I_p \cdot I_p)(L \cdot I_t) + (L \cdot L)(I_p \cdot I_t)]).
\]

(4)

It is scalar and couples eight states with the same \( J_t \). In fact, it is a block diagonal matrix with two one-dimensional blocks for the states with \( J = L \pm 3/2 \) and two three-dimensional blocks for the states with \( J = L \pm 1/2 \). The matrix elements of the Hamiltonian (4) can be obtained easily by using the algebra of angular momentum, the necessary formulas can be found, for example, in [21].

Results of the numerical calculation of the effective Hamiltonian coefficients, equation (4), for a wide range of states are presented in table 1. Examples of hyperfine splitting of some levels in HT+ are given in table 2. They were
generated by a straightforward diagonalization of the effective Hamiltonian $H_{\text{eff}}$.

4. Spin-independent relativistic corrections

The leading order relativistic corrections ($R_{\infty}a^{2}$) at present are well understood and are described by the Breit–Pauli Hamiltonian. Here we present in explicit form expressions for different terms, which contribute to this order.

The major contribution comes from the relativistic correction for the bound electron,

$$E_{\text{rc}}^{(2)} = \alpha^{2} \left( -\frac{P_{i}^{4}}{8m_{e}^{4}} + \frac{4\pi}{8m_{e}^{4}} \left[ Z_{1}\delta(r_{1}) + Z_{2}\delta(r_{2}) \right] \right).$$

(5)

The other corrections are due to a finite mass of nuclei and are called the recoil corrections of orders $R_{\infty}a^{2}(m/M)$, $R_{\infty}a^{2}(m/M)^{2}$, etc. The most important is the transverse photon exchange.
Table 3. Mean values of the various operators for the ro-vibrational states in the $^{1+}$ molecular ion.

<table>
<thead>
<tr>
<th>$L$</th>
<th>$v$</th>
<th>$(\langle r_{ph} \rangle)$</th>
<th>$(\langle r_{nuc} \rangle)$</th>
<th>$(\langle P_{d} \rangle)$</th>
<th>$(\langle P_{d} \rangle)$</th>
<th>$R_{de}$</th>
<th>$R_{pe}$</th>
<th>$R_{pd}$</th>
</tr>
</thead>
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<tr>
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<td>0</td>
<td>0.207 565 844</td>
<td>0.207 158 825</td>
<td>0.207 565 844</td>
<td>0.207 158 825</td>
<td>116.687</td>
<td>116.581</td>
<td>1.17610</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0.203 072 771</td>
<td>0.202 657 365</td>
<td>0.203 072 771</td>
<td>0.202 657 365</td>
<td>507.168</td>
<td>506.747</td>
<td>1.154 16</td>
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<tr>
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<td>2</td>
<td>0.198 859 334</td>
<td>0.198 433 353</td>
<td>0.198 859 334</td>
<td>0.198 433 353</td>
<td>1184.644</td>
<td>1183.703</td>
<td>1.133 71</td>
</tr>
<tr>
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<td>3</td>
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<td>0.194 471 883</td>
<td>0.194 911 008</td>
<td>0.194 471 883</td>
<td>2072.077</td>
<td>2070.463</td>
<td>1.114 68</td>
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<tr>
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<td>0.190 395 843</td>
<td>0.190 759 483</td>
<td>0.190 395 843</td>
<td>3011.775</td>
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<tr>
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<td>0.187 428 004</td>
<td>0.187 783 240</td>
<td>0.187 428 004</td>
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<td>4238.203</td>
<td>1.080 70</td>
</tr>
<tr>
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<td>0.184 364 389</td>
<td>0.184 704 201</td>
<td>0.184 364 389</td>
<td>2101.347</td>
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<td>1.077 09</td>
</tr>
<tr>
<td>0</td>
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<td>0.181 381 794</td>
<td>0.181 711 525</td>
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<td>3135.223</td>
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<tr>
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<td>0.178 443 897</td>
<td>0.178 751 230</td>
<td>0.178 443 897</td>
<td>4250.240</td>
<td>4246.993</td>
<td>1.080 13</td>
</tr>
</tbody>
</table>

This correction is defined (both for proton and triton) by

\[
E_{\text{corr}} = E_{\text{nuc}}^2 + E_{\text{tr-ph}}^2 + E_{\text{Darwin}} + E_{\text{nuc}}^2
\]

(10)

Results of the numerical calculation of the mean values of various operators encountered in the formulas of the previous sections are presented in table 3. We use the following notation for the transverse photon exchange contributions:

\[
R_{\text{ne}} = \frac{\langle P_{D} \rangle}{r_n} + \frac{\langle r_{ph} \rangle}{r_n}
\]

\[
R_{\text{nm}} = \frac{\langle P_{D} \rangle}{R} + \frac{\langle R_{d} \rangle}{R}
\]

(11)

These data are presented in the last three columns of the table.
Acknowledgments

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References

[23] Angeli I 2004 At. Data Nucl. Data Tables 87 185