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

A K Bekbaev[1], **V I Korobov**[2] **and M Dineykhan**[1,2]

[1] Faculty of Physics and Technology, Al-Farabi Kazakh National University, 050012, Almaty, Kazakhstan
[2] Joint Institute for Nuclear Research, 141980, Dubna, Russia

E-mail: korobov@theor.jinr.ru

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.

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[3] D M Bishop presented some evaluations of the leading order relativistic and radiative corrections based on the Born–Oppenheimer approximation.

## 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:

$$\Psi_{LM}^{\pi}(\mathbf{R}, \mathbf{r}_1) = \sum_{l_1+l_2=L} \mathcal{Y}_{LM}^{l_1 l_2}(\hat{\mathbf{R}}, \hat{\mathbf{r}}_1) G_{l_1 l_2}^{L\pi}(R, r_1, r_2),$$

$$G_{l_1 l_2}^{L\pi}(R, r_1, r_2) = \sum_{n=1}^{N} \{ C_n \operatorname{Re}[e^{-\alpha_n R - \beta_n r_1 - \gamma_n r_2}] + D_n \operatorname{Im}[e^{-\alpha_n R - \beta_n r_1 - \gamma_n r_2}] \}, \quad (1)$$
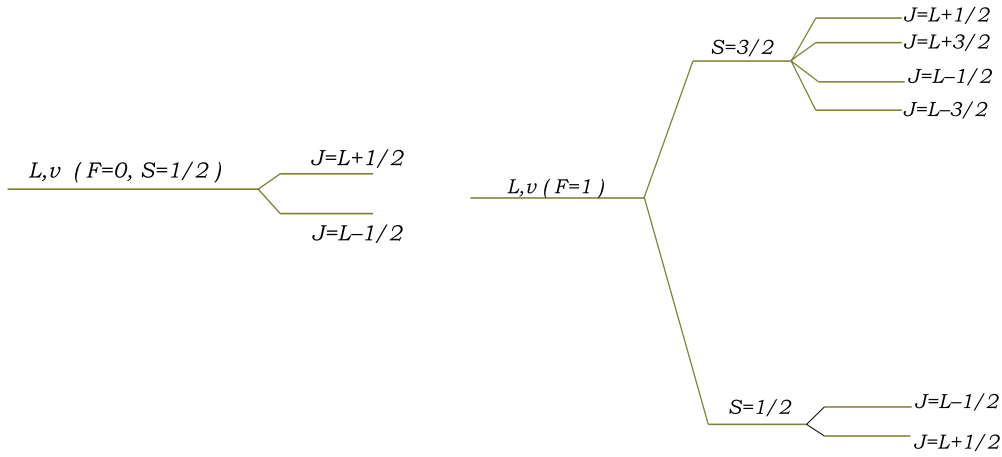
Figure 1. Schematic diagram of the HFS of the HT$^+$ molecular ion.

where the complex exponents, α, β and γ, are generated in a pseudorandom way.

When exponents α_n, β_n and γ_n 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, $M_p = 1836.152\,672\,47\,m_e$ and $M_t = 5496.921\,5269\,m_e$.

The leading correction to the nonrelativistic energy is the α^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 Hamilton for a system of particles of spin 1/2 has the following form:

$$H_{\text{HFS}} = -\frac{e^2}{c^2} \sum_{j \neq i} \frac{Z_i Z_j c_S^{(j)} [\mathbf{r}_{ij} \times \mathbf{p}_j] \mathbf{s}_j}{2m_j^2 r_{ij}^3}$$
$$- \frac{e^2}{c^2} \sum_{i>j} \frac{Z_i Z_j (c_F^{(i)} [\mathbf{r}_{ij} \times \mathbf{p}_j] \mathbf{s}_i - c_F^{(j)} [\mathbf{r}_{ij} \times \mathbf{p}_i] \mathbf{s}_j)}{m_i m_j r_{ij}^3}$$
$$+ \sum_{i>j} \left\{ \left[\frac{\boldsymbol{\mu}_i \boldsymbol{\mu}_j}{r_{ij}^3} - 3 \frac{(\boldsymbol{\mu}_i \mathbf{r}_{ij})(\boldsymbol{\mu}_j \mathbf{r}_{ij})}{r_{ij}^5} \right] - \frac{8\pi}{3} \boldsymbol{\mu}_i \boldsymbol{\mu}_j \delta(\mathbf{r}_{ij}) \right\}. \quad (2)$$

Here $\boldsymbol{\mu}_i = \left(c_F^{(i)} Z_i / 2m_i c \right) \boldsymbol{\sigma}_i$ is an operator of magnetic moment, coefficients c_F and c_S are defined

$$c_F^{(i)} = 1 + \kappa_i, \qquad c_S^{(i)} = 1 + 2\kappa_i,$$

where κ_i is an anomalous magnetic moment of a particle.

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

$$\mu_p = 2.792\,847\,337\mu_N, \qquad \mu_t = 2.978\,962\,448\mu_N$$
$$\mu_e = -1.001\,159\,652\,186\mu_B.$$

Anomalous magnetic moment κ_t for the triton may be expressed using our notations: $\kappa_t = \mu_t(m_p/m_t) - 1$.

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:

$$\mathbf{F} = \mathbf{I}_p + \mathbf{I}_t \qquad \mathbf{S} = \mathbf{F} + \mathbf{s}_e \qquad \mathbf{J} = \mathbf{S} + \mathbf{L}. \quad (3)$$

Operators $\mathbf{F}$ and $\mathbf{S}$ do not commute with the Hamiltonian, but still provide good approximate quantum numbers to describe HFS states of the system. Operator $\mathbf{F}$ 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):

$$H_{\text{eff}} = E_1(\mathbf{s}_e \cdot \mathbf{I}_p) + E_2(\mathbf{s}_e \cdot \mathbf{I}_t) + E_3(\mathbf{s}_e \cdot \mathbf{L})$$
$$+ E_4(\mathbf{I}_p \cdot \mathbf{L}) + E_5(\mathbf{I}_t \cdot \mathbf{L}) + E_6\{2L(L+1)(\mathbf{s}_e \cdot \mathbf{I}_p)$$
$$- 3[(\mathbf{L} \cdot \mathbf{s}_e)(\mathbf{L} \cdot \mathbf{I}_p) + (\mathbf{L} \cdot \mathbf{I}_p)(\mathbf{L} \cdot \mathbf{s}_e)]\} + E_7\{2L(L+1)(\mathbf{s}_e \cdot \mathbf{I}_t)$$
$$- 3[(\mathbf{L} \cdot \mathbf{s}_e)(\mathbf{L} \cdot \mathbf{I}_t) + (\mathbf{L} \cdot \mathbf{I}_t)(\mathbf{L} \cdot \mathbf{s}_e)]\} + E_8\{2L(L+1)(\mathbf{I}_p \cdot \mathbf{I}_t)$$
$$- 3[(\mathbf{L} \cdot \mathbf{I}_p)(\mathbf{L} \cdot \mathbf{I}_t) + (\mathbf{L} \cdot \mathbf{I}_t)(\mathbf{L} \cdot \mathbf{I}_p)]\}. \quad (4)$$

It is scalar and couples eight states with the same J_z. 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 spitting of some levels in HT$^+$ are given in table 2. They were

Table 1. Coefficients E_i of the effective spin Hamiltonian (4) (in MHz), $a[b] = a \times 10^b$.

L	v	E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8
0	0	925.975	989.623	–	–	–	–	–	–
0	1	905.854	968.201	–	–	–	–	–	–
0	2	886.974	948.112	–	–	–	–	–	–
0	3	869.266	929.288	–	–	–	–	–	–
0	4	852.672	911.665	–	–	–	–	–	–
0	5	837.137	895.190	–	–	–	–	–	–
1	0	925.239	988.838	28.4945	−0.278 96[−1]	−0.298 30[−1]	8.627 53	9.201 63	−0.212 74[−1]
1	1	905.157	967.457	27.0613	−0.271 48[−1]	−0.291 25[−1]	8.178 89	8.723 05	−0.205 40[−1]
1	2	886.313	947.408	25.6832	−0.263 63[−1]	−0.283 67[−1]	7.748 51	8.263 96	−0.198 01[−1]
1	3	868.641	928.621	24.3546	−0.255 43[−1]	−0.275 59[−1]	7.334 57	7.822 40	−0.190 56[−1]
1	4	852.081	911.035	23.0698	−0.246 88[−1]	−0.267 04[−1]	6.935 32	7.396 50	−0.183 04[−1]
1	5	836.578	894.595	21.8234	−0.237 98[−1]	−0.258 01[−1]	6.549 08	6.984 49	−0.175 44[−1]
2	0	923.774	987.274	28.3806	−0.277 33[−1]	−0.296 47[−1]	2.047 83	2.184 10	−0.503 83[−2]
2	1	903.768	965.976	26.9522	−0.269 86[−1]	−0.289 43[−1]	1.941 29	2.070 45	−0.486 40[−2]
2	2	884.997	946.005	25.5787	−0.262 03[−1]	−0.281 86[−1]	1.839 09	1.961 42	−0.468 84[−2]
2	3	867.395	927.294	24.2544	−0.253 85[−1]	−0.273 80[−1]	1.740 77	1.856 55	−0.451 15[−2]
2	4	850.903	909.780	22.9736	−0.245 32[−1]	−0.265 27[−1]	1.645 93	1.755 38	−0.433 30[−2]
2	5	835.466	893.410	21.7310	−0.236 46[−1]	−0.256 27[−1]	1.554 18	1.657 51	−0.415 27[−2]
3	0	921.593	984.948	28.2112	−0.274 92[−1]	−0.293 76[−1]	0.951 24	1.014 54	−0.233 25[−2]
3	1	901.701	963.772	26.7900	−0.267 47[−1]	−0.286 73[−1]	0.901 72	0.961 72	−0.225 15[−2]
3	2	883.040	943.919	25.4234	−0.259 66[−1]	−0.279 19[−1]	0.854 21	0.911 03	−0.216 99[−2]
3	3	865.543	925.320	24.1054	−0.251 51[−1]	−0.271 15[−1]	0.808 50	0.862 27	−0.208 77[−2]
3	4	849.151	907.914	22.8306	−0.243 01[−1]	−0.262 65[−1]	0.764 39	0.815 22	−0.200 47[−2]
3	5	833.811	891.649	21.5935	−0.234 18[−1]	−0.253 69[−1]	0.721 72	0.769 70	−0.192 10^{−2}
4	0	918.717	981.881	27.9879	−0.271 75[−1]	−0.290 21[−1]	0.552 52	0.589 28	−0.134 88[−2]
4	1	898.977	960.867	26.5763	−0.264 33[−1]	−0.283 20[−1]	0.523 73	0.558 57	−0.130 17[−2]
4	2	880.460	941.168	25.2186	−0.256 55[−1]	−0.275 68[−1]	0.496 10	0.529 10	−0.125 43[−2]
4	3	863.101	922.718	23.9090	−0.248 44[−1]	−0.267 68[−1]	0.469 52	0.500 74	−0.120 65[−2]
4	4	846.843	905.456	22.6421	−0.239 99[−1]	−0.259 23[−1]	0.443 86	0.473 38	−0.115 83[−2]
4	5	831.631	889.328	21.4124	−0.231 21[−1]	−0.250 32[−1]	0.419 03	0.446 89	−0.110 96[−2]
5	0	915.173	978.101	27.7131	−0.267 88[−1]	−0.285 86[−1]	0.360 85	0.384 87	−0.876 06[−3]
5	1	895.620	957.287	26.3132	−0.260 49[−1]	−0.278 87[−1]	0.342 03	0.364 79	−0.845 26[−3]
5	2	877.282	937.780	24.9665	−0.252 75[−1]	−0.271 39[−1]	0.323 96	0.345 51	−0.814 27[−3]
5	3	860.094	919.514	23.6673	−0.244 68[−1]	−0.263 44[−1]	0.306 57	0.326 96	−0.783 06[−3]
5	4	844.000	902.428	22.4101	−0.236 29[−1]	−0.255 04[−1]	0.289 79	0.309 06	−0.751 58[−3]
5	5	828.947	886.472	21.1895	−0.227 57[−1]	−0.246 19[−1]	0.273 54	0.291 72	−0.719 79[−3]

Table 2. Hyperfine splitting (in MHz) of ro-vibrational levels of the HT$^+$ molecular ion.

		$(F, S) = (0, 1/2)$		$(1, 1/2)$		$(1, 3/2)$			
L	v	$J = L − 1/2$	$L + 1/2$	$L − 1/2$	$L + 1/2$	$L − 3/2$	$L − 1/2$	$L + 1/2$	$L + 3/2$
0	0	–	0.7924	−958.592	–	–			478.900
0	1	–	0.7772	−937.805	–	–			468.514
0	2	–	0.7632	−918.306	–	–			458.772
1	0	−27.692	15.024	−949.813	−962.670	–	411.811	504.742	483.834
1	1	−26.274	14.292	−929.422	−941.678	–	404.831	492.995	473.215
1	2	−24.909	13.590	−910.305	−921.982	–	398.360	481.947	463.248
2	0	−41.746	29.141	390.895	−943.956	−966.160	451.293	505.120	493.405
2	1	−39.620	27.699	385.019	−923.854	−944.988	442.245	493.353	482.312
2	2	−37.575	26.313	379.608	−905.016	−925.119	433.791	482.286	471.888

generated by a straightforward diagonalization of the effective Hamiltonian H_{eff}.

4. Spin-independent relativistic corrections

The leading order relativistic corrections ($R_\infty \alpha^2$) 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,

$$E_{\text{rc}}^{(2)} = \alpha^2 \left\langle -\frac{\mathbf{p}_e^4}{8m_e^3} + \frac{4\pi}{8m_e^2} [Z_1 \delta(\mathbf{r}_1) + Z_2 \delta(\mathbf{r}_2)] \right\rangle. \quad (5)$$

The other corrections are due to a finite mass of nuclei and are called the recoil corrections of orders $R_\infty \alpha^2 (m/M)$, $R_\infty \alpha^2 (m/M)^2$, etc. The most important is the transverse photon exchange,

Table 3. Mean values of the various operators for the ro-vibrational states in the HT$^+$ molecular ion.

L	v	$\langle \mathbf{p}_e^4 \rangle$	$\langle \delta(\mathbf{r}_d) \rangle$	$\langle \delta(\mathbf{r}_p) \rangle$	$\langle \mathbf{P}_d^4 \rangle$	$\langle \mathbf{P}_p^4 \rangle$	R_{de}	R_{pe}	R_{pd}
0	0	6.305 464 90	0.207 565 844	0.207 158 825	116.687	116.581	1.176 10	1.170 99	5.694 59
0	1	6.171 775 94	0.203 072 771	0.202 657 365	507.168	506.747	1.154 16	1.144 23	16.161 21
0	2	6.046 817 75	0.198 859 334	0.198 433 353	1184.644	1183.703	1.133 71	1.119 48	25.282 51
0	3	5.930 146 21	0.194 911 008	0.194 471 883	2072.077	2070.463	1.114 68	1.096 66	33.154 79
0	4	5.821 365 22	0.191 214 816	0.190 759 483	3101.775	3099.388	1.097 02	1.075 69	39.862 37
0	5	5.720 123 22	0.187 759 240	0.187 283 983	4214.043	4210.823	1.080 70	1.056 48	45.478 76
1	0	6.300 342 39	0.207 401 110	0.206 994 092	123.049	122.937	1.175 32	1.170 02	5.930 45
1	1	6.166 928 14	0.202 916 687	0.202 501 247	523.105	522.671	1.153 42	1.143 31	16.369 42
1	2	6.042 232 95	0.198 711 525	0.198 285 467	1208.142	1207.182	1.133 01	1.118 63	25.465 05
1	3	5.925 814 20	0.194 771 138	0.194 331 895	2101.347	2099.711	1.114 02	1.095 86	33.313 39
1	4	5.817 276 71	0.191 082 588	0.190 627 085	3135.223	3132.811	1.096 41	1.074 94	39.998 56
1	5	5.716 270 52	0.187 634 389	0.187 158 917	4250.240	4246.993	1.080 12	1.055 78	45.593 84
2	0	6.300 342 39	0.207 401 110	0.206 994 092	123.049	122.937	1.175 32	1.170 02	5.930 45
2	1	6.166 928 14	0.202 916 687	0.202 501 247	523.105	522.671	1.153 42	1.143 31	16.369 42
2	2	6.042 232 95	0.198 711 525	0.198 285 467	1208.142	1207.182	1.133 01	1.118 63	25.465 05
2	3	5.925 814 20	0.194 771 138	0.194 331 895	2101.347	2099.711	1.114 02	1.095 86	33.313 39
2	4	5.817 276 71	0.191 082 588	0.190 627 085	3135.223	3132.811	1.096 41	1.074 94	39.998 56
2	5	5.716 270 52	0.187 634 389	0.187 158 917	4250.240	4246.993	1.080 12	1.055 78	45.593 84
3	0	6.274 981 58	0.206 585 325	0.206 178 304	161.723	161.576	1.171 46	1.165 23	7.090 63
3	1	6.142 930 36	0.202 143 824	0.201 728 208	608.785	608.283	1.149 78	1.138 81	17.392 49
3	2	6.019 540 36	0.197 979 722	0.197 553 294	1330.852	1329.796	1.129 57	1.114 39	26.360 83
3	3	5.904 375 32	0.194 078 739	0.193 638 888	2252.222	2250.471	1.110 78	1.091 88	34.090 50
3	4	5.797 045 83	0.190 428 115	0.189 971 720	3306.357	3303.815	1.093 36	1.071 21	40.664 53
3	5	5.697 207 03	0.187 016 554	0.186 539 808	4434.548	4431.162	1.077 26	1.052 30	46.155 20
4	0	6.254 990 30	0.205 942 008	0.205 534 974	200.599	200.420	1.168 41	1.161 45	7.996 30
4	1	6.124 017 24	0.201 534 462	0.201 118 695	684.241	683.679	1.146 90	1.135 25	18.189 85
4	2	6.001 659 67	0.197 402 846	0.196 976 105	1435.011	1433.876	1.126 86	1.111 05	27.057 63
4	3	5.887 486 27	0.193 533 034	0.193 092 680	2378.089	2376.242	1.108 22	1.088 75	34.693 55
4	4	5.781 112 44	0.189 912 420	0.189 455 292	3447.688	3445.039	1.090 95	1.068 28	41.179 79
4	5	5.682 198 18	0.186 529 848	0.186 052 105	4585.743	4582.243	1.075 00	1.049 56	46.587 82
5	0	6.230 364 09	0.205 149 225	0.204 742 164	258.613	258.385	1.164 65	1.156 80	9.101 15
5	1	6.100 723 66	0.200 783 653	0.200 367 684	786.718	786.076	1.143 35	1.130 88	19.160 99
5	2	5.979 642 32	0.196 692 198	0.196 265 051	1572.244	1571.003	1.123 51	1.106 94	27.904 64
5	3	5.866 695 12	0.192 860 930	0.192 419 933	2541.445	2539.474	1.105 07	1.084 90	35.424 85
5	4	5.761 503 30	0.189 277 430	0.188 819 374	3629.462	3626.675	1.087 99	1.064 67	41.802 71
5	5	5.663 731 96	0.185 930 708	0.185 451 691	4779.021	4775.376	1.072 22	1.046 19	47.108 72

$$E_{\text{tr}-\text{ph}}^{(2)} = \frac{\alpha^2 Z_1}{2m_e M_1} \left\langle \frac{\mathbf{p}_e \mathbf{P}_1}{r_1} + \frac{\mathbf{r}_1 (\mathbf{r}_1 \mathbf{p}_e) \mathbf{P}_1}{r_1^3} \right\rangle$$
$$+ \frac{\alpha^2 Z_2}{2m_e M_2} \left\langle \frac{\mathbf{p}_e \mathbf{P}_2}{r_2} + \frac{\mathbf{r}_2 (\mathbf{r}_2 \mathbf{p}_e) \mathbf{P}_2}{r_2^3} \right\rangle$$
$$- \frac{\alpha^2 Z_1 Z_2}{2M_1 M_2} \left\langle \frac{\mathbf{P}_1 \mathbf{P}_2}{R} + \frac{\mathbf{R}(\mathbf{R} \mathbf{P}_1) \mathbf{P}_2}{R^3} \right\rangle. \quad (6)$$

The contribution of the last term in (6) is not negligible and amounts to about 10% of $E_{\text{tr}-\text{ph}}^{(2)}$.

The next is the relativistic kinetic energy ($E_{\text{kin}} = \sqrt{m^2 + p^2} \approx m + p^2/2m + \dots$) correction for heavy particles,

$$E_{\text{kin}}^{(2)} = -\alpha^2 \left\langle \frac{\mathbf{P}_1^4}{8M_1^3} + \frac{\mathbf{P}_2^4}{8M_2^3} \right\rangle. \quad (7)$$

Beyond that, in the $R_\infty \alpha^2$ order, one has to consider the nuclear spin-dependent recoil corrections. For the proton (triton), spin 1/2 point-like particle, one has

$$E_{\text{Darwin}}^{(2)} = \frac{\alpha^2 \pi Z_1}{2M_1^2} \langle \delta(\mathbf{r}_1) \rangle + \frac{\alpha^2 \pi Z_2}{2M_2^2} \langle \delta(\mathbf{r}_2) \rangle. \quad (8)$$

It is convenient and important at this order ($R_\infty \alpha^2$) to also consider the finite size electromagnetic structure of nuclei.

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

$$E_{\text{nuc}}^{(2)} = \frac{2\pi Z_1 (R_1/a_0)^2}{3} \langle \delta(\mathbf{r}_1) \rangle + \frac{2\pi Z_2 (R_2/a_0)^2}{3} \langle \delta(\mathbf{r}_2) \rangle, \quad (9)$$

where R is the root-mean-square (RMS) radius of the nuclear electric charge distribution. The RMS radius for the proton is $R_p = 0.8775(51)$ fm [22], and for the triton $R_t = 1.759(36)$ fm [23]. These contributions are of comparable size (or even larger) with the Darwin contribution.

The complete contribution to this order is thus

$$E_{\alpha^2} = E_{\text{rc}}^{(2)} + E_{\text{kin}}^{(2)} + E_{\text{tr}-\text{ph}}^{(2)} + E_{\text{Darwin}}^{(2)} + E_{\text{nuc}}^{(2)}. \quad (10)$$

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:

$$R_{ne} = -\left\langle \frac{\mathbf{p}_e \mathbf{P}_n}{r_n} + \frac{\mathbf{r}_n (\mathbf{r}_n \mathbf{p}_e) \mathbf{P}_n}{r_n^3} \right\rangle,$$
$$R_{nn} = -\left\langle \frac{\mathbf{P}_1 \mathbf{P}_2}{R} + \frac{\mathbf{R}(\mathbf{R} \mathbf{P}_1) \mathbf{P}_2}{R^3} \right\rangle. \quad (11)$$

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

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