Hyperfine structure splitting of the bound $S(L = 0)$–states in the symmetric muonic molecular ions

Alexei M. Frolov

Department of Chemistry
University of Western Ontario,
London, Ontario N6H 5B7, Canada

(Dated: May 22, 2012)

Abstract

The hyperfine structure splittings are determined for all five bound $S(L = 0)$–states in the three symmetric muonic molecular ions: $pp\mu, dd\mu$ and $tt\mu$. The expectation values of all inter-particle delta-functions used in our calculations have been determined in recent highly accurate computations.
In our earlier study [1] we analyzed the hyperfine structure splitting of the bound \( S(L = 0) \)–states in the muonic molecular ions: \( pd\mu, pt\mu \) and \( dt\mu \). The main goal of this work is to consider the hyperfine structure splitting in the symmetric muonic molecular ions \( pp\mu, dd\mu \) and \( tt\mu \). Here and everywhere below in this study the notation \( p \) designates the proton, \( d \) means deuteron (the nucleus of deuterium) and \( t \) stands for the triton (or the nucleus of tritium). As is well known there are five bound \( S(L = 0) \)–states in these (symmetric) muonic molecular ions. The ground states are stable in each of these ions, while the excited \( S(L = 0) \)–states are stable only in the heavy \( dd\mu \) and \( tt\mu \) ions. In general, the analysis of the hyperfine structure in the symmetric muonic molecular ions is slightly more complicated than analogous analysis for the non-symmetric ions. On the other hand, the hyperfine structures of the symmetric muonic molecular ions are relatively simple and can be explained by using a few transparent physical ideas.

The general formula for the hyperfine structure splitting (or hyperfine splitting, for short) for an arbitrary (symmetric) three-body muonic molecular ion \( aa\mu \) is written in the following form (in atomic units) (see, e.g., [2])

\[
(\Delta H)_{\text{h.s.}} = \frac{2\pi}{3} \alpha^2 \frac{g_a g_a}{m_p^2} \langle \delta(r_{aa}) \rangle (s_a \cdot s_a) + \frac{2\pi}{3} \alpha^2 \frac{g_a g_{\mu}}{m_p m_\mu} \langle \delta(r_{a\mu}) \rangle (s_a \cdot s_{\mu}) + \frac{2\pi}{3} \alpha^2 \frac{g_{\mu} g_{\mu}}{m_p m_\mu} \langle \delta(r_{a\mu}) \rangle (S_{aa} \cdot s_{\mu})
\]

(1)

where \( \alpha = \frac{e^2}{\hbar c} \) is the fine structure constant, \( m_\mu \) and \( m_p \) are the muon and proton masses, respectively. The factors \( g_\mu \) and \( g_a \) are the corresponding \( g \)–factors. The expression, Eq. (1), for \( (\Delta H)_{\text{h.s.}} \) is, in fact, an operator in the total spin space which has the dimension \( (2s_a + 1)(2s_\mu + 1) \). Since the second and third terms in Eq.(1) are identical, then we can reduce Eq.(1) to the form

\[
(\Delta H)_{\text{h.s.}} = \frac{2\pi}{3} \alpha^2 \frac{g_a g_a}{m_p^2} \langle \delta(r_{aa}) \rangle (s_a \cdot s_a) + \frac{2\pi}{3} \alpha^2 \frac{g_a g_{\mu}}{m_p m_\mu} \langle \delta(r_{a\mu}) \rangle (S_{aa} \cdot s_{\mu})
\]

(2)

where \( S_{aa} = (s_a + s_a) \) is the total spin of the pair of identical particles, i.e. the two nuclei of the hydrogen isotopes \( (a = p, d \) and/or \( t) \).

The formula, Eq.(2), allows one to make a few qualitative predictions about the hyperfine structure of the symmetric muonic molecular ions. First, it is clear that the classifications of the levels of hyperfine structure must be based on the total spin of the two ‘symmetric’ nuclei \( S_{aa} \). The absolute values of the spin \( S_{aa} \) are always non-negative integer numbers,
i.e. \(|S_{aa}| = 0, 1, 2, \ldots\). For instance, in the case of two protons \(p\) and/or two tritons \(t\) one finds \(|S_{aa}| = 0, 1\), while for the two deuterons \(|S_{aa}| = 0, 1, 2\). The energy of the hyperfine state with \(S_{aa} = 0\) is determined only by the first term in Eq.(2). It is clear that such an energy is very small, since the expectation values \(\langle \delta(r_{aa}) \rangle\) in all muonic molecular ions are very small. As follows from actual computations of muonic molecular ions all these values are less than \(4 \cdot 10^{-5}\) (in muon atomic units), while the expectation values of the muon-nuclear delta-functions are in \(10^4 - 10^6\) times larger. Briefly, we can say that the energy of this hyperfine state (with \(J = \frac{1}{2}\) for the \(pp\mu\) and \(tt\mu\) ions) is determined by the spin-spin interaction between the two heavy nuclei (muon’s spin does not contribute). The overall contribution from the first term in Eq.(2) rapidly (exponentially) decreases when the mass of the heavy particle increases. Formally, the first term in Eq.(2) is very small already for the \(pp\mu\) ion. However, for the \(dd\mu\) and \(tt\mu\) ions its contribution is negligible. This means that in the first approximation the hyperfine structure of the symmetric muonic molecular ions can be explained by using only one term for the muon-nuclear spin-spin interaction. This leads to some ‘additional’ symmetry observed for the actual levels of hyperfine structure of heavy \(dd\mu\) and \(tt\mu\) ions (see below).

As is well known the spin of the negatively charged muon \(\mu^-\) equals \(\frac{1}{2}\) and the spins of the proton \(p\) and triton \(t\) also equal \(\frac{1}{2}\). Therefore, the hyperfine structure of the \(pp\mu\) and \(tt\mu\) ions must include eight levels which form three following groups: (1) the group of four spin states with \(J = \frac{3}{2}\), (2) the upper group of two states with \(J = \frac{1}{2}\) and (3) the lower group of two states with \(J = \frac{1}{2}\). The hyperfine energy of one of the two groups of states with \(J = \frac{1}{2}\) is very close to zero. The same classification of the hyperfine structure levels is true for the excited \(S(L = 0)\)–state in the \(tt\mu\) ion. Here and everywhere below the notation \(J\) stands for the total spin (or total momentum \(J = L + S = S = S_{aa} + s_\mu\), for the \(S(L = 0)\)–states) of the three-body ion.

The hyperfine structure of the \(dd\mu\) ion is substantially different. In the \(dd\mu\) ion one finds eighteen levels of hyperfine structure which are separated into five different groups: one group with \(J = \frac{5}{2}\) (six states), two different groups of states (upper and lower groups) with \(J = \frac{3}{2}\) (four states in each), two different groups of states (upper and lower groups) with \(J = \frac{1}{2}\) (two states in each).

In our calculations we have used the following numerical values for the constants and factors in Eq.(2): \(\alpha = 7.297352586 \cdot 10^{-3}\), \(g_\mu = -2.0023218396\) [3] and \(m_p = \ldots\)
1836.152701m_e, m_\mu = 206.768262m_e. The g-factors for the proton, deuteron and triton are determined from the formulas: 
\[ g_p = \frac{M_p}{I_p}, g_d = \frac{M_d}{I_d} \text{ and } g_t = \frac{M_t}{I_t}, \]
where \( M_p = 2.792847386, M_d = 0.857438230 \) and \( M_t = 2.97896247745 \) are the magnetic moments (in nuclear magnetons) of the proton, deuteron and triton, respectively. Here the spins of the proton, deuteron and triton are designated by the letter \( I \) with the corresponding index: \( I_p = \frac{1}{2}, I_d = 1 \) and \( I_t = \frac{1}{2} \). In Eqs. (1) - (2) these values are designated differently. In highly accurate computations of the expectation values of delta-functions we have used the following masses of the deuteron and triton: \( m_d = 3680.483014 \) m\( \text{e} \) and \( m_t = 5496.92158 \) m\( \text{e} \). These masses are often used in modern highly accurate calculations of muonic molecular ions (see, e.g., [4]).

The convergence of the expectation values of the nuclear-nuclear (or \( pp^- \)) and nuclear-muonic (or \( p\mu^- \)) delta-functions is illustrated in Table I for the \( pp\mu \) ion. The convergence of these expectation values computed for other bound \( S(L = 0) \)-states in the \( dd\mu \) and \( tt\mu \) ions is very similar to the results presented in Table I for the \( pp\mu \) ion. The hyperfine structure and energy splittings between the corresponding levels for all five bound \( S(L = 0) \)-states in the three muonic molecular ions \( pp\mu, dd\mu \) and \( tt\mu \) can be found in Tables II and III. In atomic physics these values are traditionally given in MHz. The corresponding conversion factor is \( 6.57968392061 \times 10^9 \) MHz/a.u. In Tables II and III the excited states are designated by the asterisk used as the upper index, e.g., \((dd\mu)^*\) and \((tt\mu)^*\). Such a system of notation is often used for muonic molecular ions.

Tables II and III contain both the energies of the levels of hyperfine structure (\( \epsilon_J \)) and hyperfine structure splitting (\( \Delta(J_1 \rightarrow J_2) \)). As we have predicted (see above) one of the hyperfine levels has a very small energy. As follows from Tables II and III this level corresponds to \( J = \frac{1}{2} \). In the \( tt\mu \) ion the hyperfine energies of this state are \( \approx 11.0591 \) MHz and \( \approx 12.4307 \) MHz for the ground and first excited states, respectively. In the \( dd\mu \) ion the energies of the analogous levels are \( 6.8996 \) MHz and \( 4.7378 \) MHz, respectively. Briefly, this means that the overall contribution of the nuclear-nuclear spin interaction is very small for the both \( dd\mu \) and \( tt\mu \) ions. This directly follows from the known fact (see, e.g., [5]) that the expectation values of nuclear-nuclear delta-functions in the \( dd\mu \) and \( tt\mu \) ions are very small. For instance, for the \( dd\mu \) and \( tt\mu \) ions the expectation values of nuclear-nuclear delta-functions are
\[ \langle \delta_{dd} \rangle \approx 2.43871205 \cdot 10^{-6} \text{ (m.a.u.)}, \]
\[ \langle \delta_{dd} \rangle \approx 1.67460229 \cdot 10^{-6} \text{ (m.a.u.)}, \]
\[ \langle \delta_{tt} \rangle \approx 2.15893994 \cdot 10^{-7} \text{ (m.a.u.)} \] and \( \langle \delta_{tt} \rangle \approx 2.42670033 \cdot 10^{-7} \text{ (m.a.u.)}, \) for the ground and
excited states, respectively. Finally, the observed hyperfine structure of these two ions is mainly (99.9999 %) related to the muon-nuclear spin-spin interactions. In the \( \text{pp}\mu \) ion the situation is slightly different, but even for this ion the overall contribution of the muon-nuclear spin interaction(s) is substantially larger than the contribution from the nuclear-nuclear spin-spin interaction.

[1] A.M. Frolov, *Hyperfine structure splitting of the ground states in the \( \text{pd}\mu, \text{pt}\mu \) and \( \text{dt}\mu \) ions*, ArXiv: 1111.6351 [atom.phys; nucl.phys.] (2011).

[2] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics. Non-Relativistic Theory*, 3rd. edn. (Oxford, England, Pergamon Press (1977)).

[3] *CRC Handbook of Chemistry and Physics*, 85th Edition, Ed. D.R. Lide, (CRC Press, Inc., Boca Raton, Florida, 2004).

[4] A.M. Frolov and D.M. Wardlaw, Eur. Phys. Jour. D 63, 339 - 350 (2011).

[5] A.M. Frolov, Phys. Rev. A 59, 4479 (1999).
TABLE I: The convergence of the $\langle \delta_{p\mu} \rangle$ and $\langle \delta_{pp} \rangle$ expectation values for the ground (bound) $S(L = 0)$—state of the $pp\mu$ molecular ion (in muon-atomic units).

| $N$  | $\langle \delta_{31} \rangle$       | $\langle \delta_{21} \rangle$       |
|------|------------------------------------|------------------------------------|
| 3300 | $1.315008614364 \cdot 10^{-1}$    | $3.9370034861 \cdot 10^{-5}$       |
| 3500 | $1.315008614369 \cdot 10^{-1}$    | $3.9370034722 \cdot 10^{-5}$       |
| 3700 | $1.315008614374 \cdot 10^{-1}$    | $3.9370034782 \cdot 10^{-5}$       |
| 3840 | $1.315008614378 \cdot 10^{-1}$    | $3.9370034773 \cdot 10^{-5}$       |

TABLE II: The hyperfine structure and hyperfine structure splitting of the bound $S(L = 0)$—states of the $pp\mu$ and $tt\mu$ ions (in MHz).

|          | $pp\mu$                | $tt\mu$                | $(tt\mu)^*$                |
|----------|------------------------|------------------------|----------------------------|
| $\epsilon_{f=\frac{3}{2}}$ | $1.256448515 \cdot 10^7$ | $1.736310113 \cdot 10^7$ | $1.510018118 \cdot 10^7$ |
| $\epsilon_{f=\frac{1}{2}}$ | $1.772596177 \cdot 10^3$ | $1.105911127 \cdot 10^1$ | $1.243070661 \cdot 10^1$ |
| $\epsilon_{f=-\frac{1}{2}}$ | $-2.513074289 \cdot 10^{-7}$ | $-3.472621366 \cdot 10^{-7}$ | $-3.020037480 \cdot 10^{-7}$ |
| $\Delta(\frac{3}{2} \rightarrow \frac{1}{2})$ | $1.256271251 \cdot 10^7$ | $1.735309024 \cdot 10^7$ | $1.510016875 \cdot 10^7$ |
| $\Delta(\frac{1}{2} \rightarrow \frac{3}{2})$ | $2.513251549 \cdot 10^7$ | $3.472622472 \cdot 10^7$ | $3.020038723 \cdot 10^7$ |
TABLE III: The hyperfine structure and hyperfine structure splitting of the bound $S(L = 0)$—states of the $dd\mu$ ion (in MHz).

|            | $dd\mu$         | $(dd\mu)^*$    |
|------------|-----------------|----------------|
| $\epsilon_{J=\frac{3}{2}}$ | $4.656669271 \cdot 10^6$ | $4.023227167 \cdot 10^6$ |
| $\epsilon_{J=\frac{3}{2}}$ | $2.328339810 \cdot 10^6$ | $2.011617137 \cdot 10^6$ |
| $\epsilon_{J=\frac{5}{2}}$ | $6.899579465 \cdot 10^9$ | $4.737788941 \cdot 10^9$ |
| $\epsilon_{J=\frac{1}{2}}$ | $-4.656669271 \cdot 10^6$ | $-4.023227167 \cdot 10^6$ |
| $\epsilon_{J=\frac{1}{2}}$ | $-6.985012530 \cdot 10^6$ | $-6.034846672 \cdot 10^6$ |
| $\Delta(\frac{5}{2} \rightarrow \frac{3}{2})$ | $2.328329461 \cdot 10^6$ | $2.01161003 \cdot 10^6$ |
| $\Delta(\frac{3}{2} \rightarrow \frac{1}{2})$ | $2.328332911 \cdot 10^6$ | $2.01161239 \cdot 10^6$ |
| $\Delta(\frac{1}{2} \rightarrow \frac{1}{2})$ | $4.656676170 \cdot 10^6$ | $4.02323191 \cdot 10^6$ |
| $\Delta(\frac{1}{2} \rightarrow \frac{3}{2})$ | $2.328343259 \cdot 10^6$ | $2.01161951 \cdot 10^6$ |