Hyperfine structure splitting of the positron-helium ions $e^+[{}^{3}\mathrm{He}(2{}^{3}S)]$ and $e^+[{}^{4}\mathrm{He}(2{}^{3}S)]$

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The hyperfine structure splittings are determined for the lowest bound state in the positron-helium ion $e^+[{}^{3}\text{He}(2{}^{3}S)]$ and $e^+[{}^{4}\text{He}(2{}^{3}S)]$. In particular, we have fond that for the $e^+[{}^{3}\text{He}(2{}^{3}S)]$ ion one can observe the three following hyperfine structure splittinings: 5824.3986, 76466.5308 and 5824.4019 MHz. In the $e^+[{}^{4}\text{He}(2{}^{3}S)]$ ion only one hyperfine structure splitting 82963.0427 MHz can be observed. All these values can be measured in modern experiments.

The positron-helium ions are of some interest in Astrophysics and applications related to the positron annihilation and positron conservation in light atomic systems (see, e.g., [1-4] and references therein). In our earlier study [5] we have shown that the the positronhelium ion e^+ He is bound, if (and only if) the two of its electrons are in the triplet state. In respect with this in [5] and in this study the bound positron-helium ion is designated as $e^+[\text{He}(2^3S)]$. The expectation values of various bound state properties in this ion were presented in [5]. Since then our computational results for the $e^+[\text{He}(2^3S)]$ ion have been improved substantially. However, in this study we want to investigate the hyperfine structure and evaluate the hyperfine structure splittings for the ground bound state of the $e^{+}[\text{He}(2^{3}S)]$ ion. This problem has never been solved accurately (see discussion in [5]). On the other hand, we have found that the hyperfine structures of the $e^+[\text{He}(2^3S)]$ ions are relatively reach and due to some reasons (see below) they are very interesting objects for investigation.

The operator responsible for the hyperfine structure splitting (or hyperfine splitting, for short) in the fourbody $e^+[\text{He}(2^3S)]$ ion is written in the following form (in atomic units) (see, e.g., [5, 6])

$$\begin{aligned} (\Delta H)_{h.s} &= \frac{2\pi}{3} \alpha^2 \frac{g_{\mathrm{He}}g_-}{m_p} \langle \delta(\mathbf{r}_{\mathrm{He}-e^-}) \rangle (\mathbf{I}_{\mathrm{He}} \cdot \mathbf{S}_-) + \\ &+ \frac{2\pi}{3} \alpha^2 g_+ g_- \langle \delta(\mathbf{r}_{+-}) \rangle (\mathbf{s}_+ \cdot \mathbf{S}_-) + \\ &+ \frac{2\pi}{3} \alpha^2 \frac{g_{\mathrm{He}}g_+}{m_p} \langle \delta(\mathbf{r}_{\mathrm{He}-e^+}) \rangle (\mathbf{I}_{\mathrm{He}} \cdot \mathbf{s}_+), \end{aligned}$$
(1)

where $\alpha = e^2/\hbar c$ is the fine structure constant, m_p is the proton mass, g_{He}, g_- , and g_+ are the g-factors of the He-nucleus, electron and positron, respectively. In this equation \mathbf{S}_- is the total vector of the two-electron

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spin, \mathbf{I}_{He} is the spin of the nucleus and \mathbf{s}_+ is the positron spin. Note that the expression, Eq. (1), for $(\Delta H)_{h.s.}$ is, in fact, an operator in the total spin space which has the dimension $N = (2S_- + 1) \cdot 2(2I_{\text{He}} + 1) = 6(2I_{\text{He}} + 1)$. In the case of the ³He nucleus the dimension N equals 12, while for the ⁴He nucleus such a dimension (N) equals 6.

In our calculations we have used the following numerical values for the constants and factors in Eq. (1): $\alpha = 7.297352586 \cdot 10^{-3}, m_p = 1836.152701m_e, g_- =$ = -2.0023193043622, and $g_+ = -g_-$. The g-factor of the helium-3 nucleus is determined from the formula: $g_N = \mathcal{M}_N/I_N = -4.2555016$, where $\mathcal{M}_N =$ = -2.1277508 [7] is the magnetic moment (in nuclear magnetons) of the helium-3 nucleus. The spin of the helium-3 nucleus is $I_{\text{He}} = 1/2$. The both spin and gfactor of the helium-4 nucleus equal zero.

The diagonalization of the matrix of the $(\Delta H)_{h,s}$ operator, Eq. (1), leads to the conclusion that twelve spin states of the hyperfine structure of the $e^+[{}^{3}\text{He}(2{}^{3}S)]$ ion are separated into four different gourps which correspond to the following values of the total angular momentum J = 1, 2, 0 and 1, respectively. The total number of hyperfine states in each group equals 2J + 1. The corresponding energies of these groups of states can be found in Table. All these energies are ex-

The hyperfine structure and hyperfine structure splitting of the bound state in the $e^+[{}^{3}\mathrm{He}(2{}^{3}S)]$ ion (in MHz)

	ε_J	$\Delta_{J;J-1}$
$\epsilon_{J=1}$	31313.243034	
$\epsilon_{J=2}$	25488.844413	5824.39862
$\epsilon_{J=0}$	-50977.686376	76466.53081
$\epsilon_{J=1}$	-56802.088263	5824.40189

pressed in MHz. The differences $\Delta_{J;J-1}$ between the corresponding hyperfine energies, i.e. the values

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$$\Delta_{J;J-1} = \varepsilon_J - \varepsilon_{J-1} \tag{2}$$

are called the hyperfine structure splittings. These values can be measured in modern experiments. The coincidence of the experimental and predicted values of $\Delta_{J;J-1}$ can be used to confirm the actual creation of the $e^{+}[{}^{3}\text{He}(2{}^{3}S)]$ ion. For the $e^{+}[{}^{3}\text{He}(2{}^{3}S)]$ ion we have found the three following splittinings: $\Delta_{1,2} \approx$ ≈ 5824.3986 MHz, $\Delta_{2:0} \approx 76466.5308$ MHz, and $\Delta_{0:1} \approx$ $\approx 5824.4019 \text{ MHz}$. Note that the values $\Delta_{1,2}$ and $\Delta_{0,1}$ almost coincide with each other. Formally, it follows from the fact that spin-spin interaction between the positron and ³He nucleus in the $e^{+ [{}^{3}\text{He}(2{}^{3}S)]}$ ion is very small (almost negligible), since the corresponding expectation value of the positron-nucleus (or positronhelium) delta-function is very small ($< 1.285 \cdot 10^{-6}$ a.u.). All our calculations for the $e^{+}[\operatorname{He}(2^{3}S)]$ ions have been performed with the use of KT-variational expansion [8] of six-dimensional gaussoids in relative four-body coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}$ (for more details see [5]). This solves the "mystery" of the hyperfine structure splitting in the $e^{+[^{3}\text{He}(2^{3}S)]}$ ion.

In the $e^{+}[{}^{4}\text{He}(2{}^{3}S)]$ ion we have six spin states which are separated into two groups: (a) four states with J = 3/2 and (b) two states with J = 1/2. The difference between these group of states is $\Delta_{3/2;1/2} \approx 55308.6951$. $\cdot 3/2 \approx 82963.0427 \,\mathrm{MHz}$. This frequency corresponds to the electron-positron spin-spin interaction. For the both $e^{+}[{}^{3}\text{He}(2{}^{3}S)]$ and $e^{+}[{}^{4}\text{He}(2{}^{3}S)]$ ions the electronpositron spin-spin interaction is the largest component of the hyperfine structure splitting. Note again that the both electrons are assumed to be in the triplet state, i.e. $S_{-} = 1$. The hyperfine structure splitting in the $e^+[{}^4\text{He}(2^3S)]$ ion is related only with the electronpositron spin-spin interaction. For the $e^{+[^{3}\text{He}(2^{3}S)]}$ ion the electron-positron spin-spin interaction is mixed with the two other components of the hyperfine structure splitting: with the electron-nuclear spin-spin interaction and with the positron-nuclear spin interaction. The resulting value of the largest component of the hyperfine structure splitting in the $e^{+}[{}^{3}\text{He}(2{}^{3}S)]$ ion decreases to 76466.5308 MHz. We can see the two other frequencies (5824.3986 and 5824.4019 MHz) which represent the hyperfine structure splitting associated mainly with the electron-nuclear spin-spin interaction in the $e^{+}[{}^{3}\text{He}(2{}^{3}S)]$ ion. These values are comparable with the analogous splitting in the triplet 2^3S -state of the ³He atom: 6740.452154 MHz (non-relativistic theory, [9]) and 6739.701177(16) MHz (experiment [10]). The difference between the two frequencies 5824.3986 and 5824.4019 MHz is very small < 30 kHz. It can be explained by the contribution from the positron-helium spin-spin interaction. In reality, such a small value is very difficult to measure. However, this value is of great interest, since it can be used as an independent measure of the accuracy of modern accurate calculations for the Coulomb four-body systems. The hyperfine structure of the excited states in the $e^{+[^{3}\text{He}(2^{3}S)]}$ and $e^{+[^{4}\text{He}(2^{3}S)]}$ ions is very similar to the hyperfine structure of the ground states in these ions described above.

- 1. R. J. Drachman, Can. J. Phys. 60, 494 (1982).
- D. M. Schrader, in: Positron Annihilation (ed. by P. G. Coleman, S. C. Sharma, and L. M. Diana), North-Holland, Amsterdam, 1982, p. 71.
- C. J. Kleinman, Y. Hahn, and L. Spurch, Phys. Rev. 165, 53 (1968).
- R. J. Drachman, Y. K. Ho, and S. K. Houston, J. Phys. B 9, L199 (1976).
- 5. A. M. Frolov, Phys. Rev. A 71, 032406 (2005).
- L. D. Landau and E. M. Lifshitz, Quantum Mechanics. Non-Relativistic Theory, 3rd. ed., Oxford, England, Pergamonn Press, 1977.
- CRC Handbook of Chemistry and Physics, 85th edition (ed. by D. R. Lide), CRC Press, Inc., Boca Raton, Florida, 2004.
- N. N. Kolesnikov and V. I. Tarasov, Yad. Fiz. 35, 609 (1982) [Sov. J. Nucl. Phys. 35, 354 (1982)].
- 9. A. M. Frolov, JCP 126, 104302 (2007).
- S.D. Rosner and A.M. Pipkin, Phys. Rev. A 1, 571 (1970).