Annihilation of the electron-positron pairs in the positronium ion Ps\(^-\) and bi-positronium Ps\(^2\).

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Abstract

Rates of the two-, three-, four- and five-photon annihilations of the electron-positron pairs are determined numerically for the three-body positronium ion Ps\(^-\) (\(e^-e^+e^-\)) and four-body bi-positronium ‘molecule’ Ps\(^2\) (\(e^-e^+e^-e^+\)). The values obtained in our computations are \(\Gamma_{2\gamma}(Ps^-) \approx 2.08048530525 \times 10^9 \text{ sec}^{-1}\), \(\Gamma_{3\gamma}(Ps^-) \approx 5.6364151550 \times 10^6 \text{ sec}^{-1}\), \(\Gamma_{4\gamma}(Ps^-) \approx 3.075 \times 10^3 \text{ sec}^{-1}\), \(\Gamma_{5\gamma}(Ps^-) \approx 5.383 \text{ sec}^{-1}\) and \(\Gamma_{2\gamma}(Ps_2) \approx 4.4385952 \times 10^9 \text{ sec}^{-1}\), \(\Gamma_{3\gamma}(Ps_2) \approx 1.202497 \times 10^7 \text{ sec}^{-1}\), \(\Gamma_{4\gamma}(Ps_2) \approx 6.562 \times 10^3 \text{ sec}^{-1}\), \(\Gamma_{5\gamma}(Ps_2) \approx 11.484 \text{ sec}^{-1}\). The four- and five-photon annihilation rates are significantly smaller than the corresponding two- and three-photon annihilation rates known for these systems. We also determine the rates of one- and zero-photon annihilation for the Ps\(^-\) ion and Ps\(^2\) system. The corresponding numerical values are \(\Gamma_{1\gamma}(Ps^-) \approx 3.82491 \times 10^{-2} \text{ sec}^{-1}\), \(\Gamma_{1\gamma}(Ps_2) \approx 1.94188 \times 10^{-1} \text{ sec}^{-1}\) and \(\Gamma_{0\gamma}(Ps_2) \approx 2.32197 \times 10^{-9} \text{ sec}^{-1}\).

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I. INTRODUCTION

In this work we consider the annihilation of electron-positron pairs (or \((e^-, e^+)\)-pairs, for short) in the three-body positronium ion \(\text{Ps}^-\) and four-body bi-positronium system (or molecule) \(\text{Ps}_2\). Our main goal is to evaluate the four- and five-photon annihilation rates in these systems. Another goal is to re-evaluate the ‘traditional’ two- and three-photon annihilation rates known for these two systems. In addition to these values we determine the one- and zero-photon annihilation rates which are also of interest in some applications. In general, the \(n\)-photon annihilation of the electron-positron pair is written in the form

\[ e^- + e^+ = \hbar \omega_1 + \hbar \omega_2 + \hbar \omega_3 + \ldots + \hbar \omega_n \]

(1)

where \(n\) is the total number of the emitted photons, \(\omega_i\) \((i = 1, \ldots, n)\) are the corresponding photon frequencies and \(\hbar \approx 1.054571628 \cdot 10^{-34} \text{ J \cdot sec}\) is the Planck constant (also called the reduced Planck constant or Dirac constant). Annihilation of electron-positron pairs from bound states of various polyelectrons is determined by the total annihilation rate \(\Gamma\) which is the sum of partial annihilation rates \(\Gamma_{n\gamma}\), i.e. \(\Gamma = \Gamma_{2\gamma} + \Gamma_{3\gamma} + \Gamma_{4\gamma} + \Gamma_{5\gamma} + \ldots\), where \(\Gamma_{n\gamma}\) is the partial \(n\)-photon annihilation rate. For some additional conditions (see below), the one-photon annihilation and zero-photon annihilation of the electron-positron pair are also possible. For different polyelectrons, different atoms and molecules which contain positrons the numerical values of \(\Gamma, \Gamma_{2\gamma}, \Gamma_{3\gamma}, \Gamma_{4\gamma}, \) etc can be substantially different. Below, we consider the annihilation of electron-positron pairs in the three-body \(\text{Ps}^-\) ion and four-body \(\text{Ps}_2\) system (bi-positronium).

II. ANNIHILATION OF THE POSITRONIUM ION

Positron annihilation in the three-body \(\text{Ps}^-\) ion was considered in a number of studies (see, e.g., [2], [3], [4] and references therein). Note that the \(\text{Ps}^-\) ion (or \(e^-e^+e^-\) ion) has only one bound state which is the singlet (ground) \(1^1S(L = 0)\)-state. It follows from here that in the \(\text{Ps}^-\) ion one electron-positron pair is always in its singlet \(1S\)-state, while second such a pair is in its triplet \(3S\)-state. Therefore, annihilation of the \((e^-, e^+)\)-pair in the \(\text{Ps}^-\) ion may proceed with the emission of an arbitrary (even or odd) number of photons. In reality, such an annihilation proceeds with the emission of the one-, two-, three- or more photons. The one-photon annihilation rate (or width) \(\Gamma_{1\gamma}\) is written in the following form \([5]\) (see also
\[ \Gamma_1 \gamma = \frac{64\pi^2}{27} \cdot \alpha^8 \cdot c \cdot a_0^{-1} \cdot \langle \delta_{321} \rangle = 1065.7569198 \cdot \langle \delta_{321} \rangle \sec^{-1}, \]

where \( \alpha = 0.7297352568 \cdot 10^{-2} \) is the fine structure constant, \( c = 0.299792458 \cdot 10^9 \text{ m} \cdot \text{sec}^{-1} \) is the velocity of light, and the Bohr radius \( a_0 \) equals 0.5291772108 \( \cdot 10^{-10} \text{ m} \). The value \( \langle \delta_{321} \rangle \) used in this formula is the expectation value of the triple delta-function computed for the ground state of the Ps\(^-\) ion. This value is the probability of finding all three particles at one spatial point. In actual computations the triple delta-function \( \delta_{321} \) is computed with the use of the following formulas

\[ \delta_{321} = \delta(r_{32})\delta(r_{21}) = \delta(r_{31})\delta(r_{21}) = \delta(r_{31})\delta(r_{32}). \]

In some works, the triple delta-function for the Ps\(^-\) ion is designated as \( \delta_{+--} \). By using the expectation value of the triple delta-function \( \langle \delta_{321} \rangle \) for the Ps\(^-\) ion from [7] one finds from the formula given above that \( \Gamma_1 \gamma \approx 3.82340 \cdot 10^{-2} \sec^{-1} \). Note that the total non-relativistic energy of the ground 1\(^1\)S\(^-\) state of the Ps\(^-\) ion obtained with the same wave function is -0.26200 50702 32980 10777 03745 a.u. It is lowest variational energy to-date.

Consider now the two- and three-photon annihilation rates in the Ps\(^-\) ion. For an arbitrary atom/molecule which contains electrons and positrons the rates of two- and three-photon annihilation of the \((e^-, e^+)\)\(^-\)pair are [7]

\[ \Gamma_2 = 4\pi\alpha^4ca_0^{-1}\left[1 - \frac{\alpha}{\pi}\left(5 - \frac{\pi^2}{4}\right)\right]\langle\delta(r_{+-})\rangle \approx 4 \cdot 50.17280269804 \cdot 10^9 \cdot \langle\delta_{+-}\rangle \sec^{-1} \quad (2) \]

and

\[ \Gamma_3 = \frac{16(\pi^2 - 9)}{9}\alpha^5ca_0^{-1}\langle\delta(r_{+-})\rangle \approx \frac{4}{3} \cdot 1.35927229774 \cdot 10^8\langle\delta_{+-}\rangle \sec^{-1} \quad (3) \]

respectively. Both these formulae explicitly contain the expectation value of the two-body electron-positron delta-function \( \delta(r_{+-}) = \delta_{+-} \). The expression for \( \Gamma_2 \gamma \), Eq.(2), also includes the lowest order radiative correction [8]. Note again that the two-photon annihilation of the \((e^-, e^+)\)\(^-\)pair proceeds only from its singlet states, while analogous three-photon annihilation is possible only from the triplet state of the electron-positron pair.

In actual applications to polyelectrons the expressions, Eqs.(2) - (3), must be multiplied by the total number of the singlet/triplet electron-positron pairs \( n \) and corresponding statistical weights of the considered singlet/triplet spin states. For the considered Ps\(^-\) ion we have \( n = 2 \), while statistical weights of the singlet and triplet states equal \( \frac{1}{4} \) and \( \frac{3}{4} \), respectively. Therefore, from the formulae presented above one finds

\[ \Gamma_2 \gamma (\text{Ps}) = n\pi\alpha^4ca_0^{-1}\left[1 - \frac{\alpha}{\pi}\left(5 - \frac{\pi^2}{4}\right)\right]\langle\delta(r_{+-})\rangle \approx 100.3456053781 \cdot 10^9\langle\delta_{+-}\rangle \sec^{-1} \quad (4) \]
\[ \Gamma_{3\gamma}(\text{Ps}^-) = n \frac{4(\pi^2 - 9)}{3} \alpha^5 \alpha_{\text{a}}^{-1} \langle \delta(r_{++}) \rangle \approx 2.718545954 \times 10^8 \langle \delta_{++} \rangle \text{sec}^{-1}, \]  

(5)

where \( \langle \delta_{++} \rangle \) is the expectation value of the electron-positron delta-function determined for the \( 1^1S \)-state in the \( \text{Ps}^- \) ion.

Now, let us discuss the multiphoton annihilation of the electron-positron pairs in the \( \text{Ps}^- \) ion. The multiphoton annihilation includes, in particular, the cases of four- and five-photon annihilation. It was shown in [1] that the rates of the four- and two-photon annihilation in the para-positronium (i.e. in the \((e^-, e^+)\)-pair in its singlet state) are related to each other by the following approximate equation

\[ \Gamma_{4\gamma}(\text{Ps}) \approx 0.274 \left( \frac{\alpha}{\pi} \right)^2 \Gamma_{2\gamma}(\text{Ps}) \]  

(6)

Since the three-body \( \text{Ps}^- \) ion contains only one singlet electron-positron pair, then from Eq.(6) one finds an analogous expression for the \( \text{Ps}^- \) ion

\[ \Gamma_{4\gamma}(\text{Ps}^-) \approx 0.274 \left( \frac{\alpha}{\pi} \right)^2 \Gamma_{2\gamma}(\text{Ps}^-) \]  

(7)

where \( \Gamma_{4\gamma}(\text{Ps}^-) \) and \( \Gamma_{2\gamma}(\text{Ps}^-) \) are the corresponding annihilation rates of the \( \text{Ps}^- \) ion. For the two-photon annihilation rate \( \Gamma_{2\gamma} \) in Eq.(7) one can use the explicit expression Eq.(4). Formally, in Eq.(7) the formula for the \( \Gamma_{2\gamma} \) rate must be used which does not contain the lowest order radiative correction. But, for approximate evaluations we can ignore such a small difference in \( \Gamma_{2\gamma} \). For the five-photon annihilation rate in the \( \text{Ps}^- \) ion one analogously finds the following result

\[ \Gamma_{5\gamma}(\text{Ps}^-) \approx 0.177 \left( \frac{\alpha}{\pi} \right)^2 \Gamma_{3\gamma}(\text{Ps}^-) \]  

(8)

This result is based on the formula from [1].

By using the formulae Eq.(7) and Eq.(8) and the numerical values of the \( \Gamma_{2\gamma} \) and \( \Gamma_{3\gamma} \) annihilation rates computed above we can evaluate the four- and five-photon annihilation rates in the \( \text{Ps}^- \) ion. The corresponding numerical values are \( \Gamma_{1\gamma} \approx 3.82491 \times 10^{-2} \text{sec}^{-1} \), \( \Gamma_{2\gamma} \approx 2.08048530525 \times 10^0 \text{sec}^{-1} \), \( \Gamma_{3\gamma} \approx 5.6364151550 \times 10^6 \text{sec}^{-1} \), \( \Gamma_{4\gamma} \approx 3.075 \times 10^3 \text{sec}^{-1} \) and \( \Gamma_{5\gamma} \approx 5.383 \text{sec}^{-1} \). The \( \Gamma_{4\gamma} \) and \( \Gamma_{5\gamma} \) rates have not been evaluated in earlier studies. The computed annihilation rates \( \Gamma_{2\gamma}, \Gamma_{3\gamma}, \Gamma_{4\gamma}, \Gamma_{5\gamma} \) and \( \Gamma_{1\gamma} \) allow one to determine the effective life-time of the \( \text{Ps}^- \) ion. The numerical computation of these annihilation rates performed in this Section essentially solves the problem of positron annihilation in the \( \text{Ps}^- \) ion. It
is interesting to note that the $\Gamma_{4\gamma}$ and $\Gamma_{5\gamma}$ annihilation rates are very small in value. By using the numerical values of all computed annihilation rates one finds that in the $\text{Ps}^-$ ion, $\Gamma_{3\gamma} \gg \Gamma_{4\gamma} \gg \Gamma_{5\gamma} \gg \Gamma_{1\gamma}$. Formally, this relationship means that the $\text{Ps}^-$ ion can essentially be described as a system with the two annihilation rates ($\Gamma_{2\gamma}$ and $\Gamma_{3\gamma}$) only. The partial annihilation probabilities are:

$$\Delta_{2\gamma} = \frac{\Gamma_{2\gamma}}{\Gamma_{2\gamma} + \Gamma_{3\gamma}} \approx 0.9973,$$

$$\Delta_{3\gamma} = \frac{\Gamma_{3\gamma}}{\Gamma_{2\gamma} + \Gamma_{3\gamma}} \approx 0.0027.$$ (9)

In other words, $\approx 99.7\%$ of all $\text{Ps}^-$ ions decay with the emission of two photons, while $\approx 0.3\%$ of these ions decay with the emission of three photons. It is interesting to note that the same situation can be found in other polyelectrons, including bi-positronium $\text{Ps}_2$, bi-positronium ion $\text{Ps}_2e^-$, etc. Each of these systems has only two annihilation channels: (a) two-photon channel and (b) three-photon channel. The rest of the annihilation channels can be ignored for all polyelectrons. This allows one to describe the annihilation of arbitrary polyelectrons and their mixtures.

### III. ANNIHILATION OF THE BI-POSITRONIUM

Annihilation of the $(e^-, e^+)$-pair in the four-body bi-positronium $\text{Ps}_2$ can proceed with the emission of one-, two-, three- and larger number of photons; yet in the bi-positronium $\text{Ps}_2$ the zero-photon annihilation is also possible. Let us present the known analytical formulae for the partial annihilation rates $\Gamma_{n\gamma}$ in bi-positronium $\text{Ps}_2$. First, consider the two-photon annihilation. The analytical expression for the two-photon annihilation rate which also includes the lowest-order radiative correction [8] takes the form

$$\Gamma_{2\gamma} = \pi \left[1 - \frac{\alpha}{\pi} \left(5 - \frac{\pi^2}{4}\right)\right] \cdot \alpha^4 \cdot n(c a_0^{-1}) \cdot \langle \delta_{+-} \rangle = 50.17280268904 \cdot 10^9 \cdot n \cdot \langle \delta_{+-} \rangle \ sec^{-1},$$ (10)

where $n$ is the total number of electron-positron pairs in polyelectron. For bi-positronium $\text{Ps}_2$ one finds $n = 2 \cdot 2 = 4$. In Eq.(10) the notation $\langle \delta_{+-} \rangle$ designates the expectation value of the electron-positron delta-function $\delta_{+-}$. It is assumed everywhere in this study that all few-particle wave functions are properly antisymmetrized upon identical particles. Now, by using our best expectation value obtained for the electron-positron delta-function $\langle \delta_{+-} \rangle \approx 2.211775 \cdot 10^{-2}$ (our method was described in [9]) one finds that $\Gamma_{2\gamma}(\text{Ps}_2) \approx 4.4385952 \cdot 10^9 sec^{-1}$. The non-relativistic energy of the ground state of the bi-positronium $\text{Ps}_2$ obtained with the same wave function is -0.5160 0379 0316 a.u.
The three-photon annihilation rate $\Gamma_{3\gamma}(Ps_2)$ can be written in the form

$$\Gamma_{3\gamma} = \frac{4}{3} (\pi^2 - 9) \alpha^5 \cdot n(ca_0^{-1}) \cdot \langle \delta_{+-} \rangle = 1.35927298 \cdot 10^7 \cdot n \cdot \langle \delta_{+-} \rangle \ sec^{-1}. \quad (11)$$

By using the same expectation value of $\langle \delta_{+-} \rangle$ one finds that $\Gamma_{3\gamma}(Ps_2) \approx 1.202497 \cdot 10^7 \ sec^{-1}$.

The one-photon ($e^-, e^+$)-pair annihilation in the bi-positronium $Ps_2$ proceeds with the emission of one fast electron or positron. Formally, in the bi-positronium we have two one-photon annihilation rates $\Gamma_1(e^-)$ and $\Gamma_1(e^+)$, where the notation $e^-/e^+$ means that the fast electron/positron is emitted during the one-photon annihilation. In actual applications we can always assume that $\Gamma_1(e^-) = \Gamma_1(e^+)$. In this case the total one-photon annihilation rate $\Gamma_1 = \Gamma_1(e^-) + \Gamma_1(e^+) = 2\Gamma_1(e^-)$ for the $Ps_2$ system is

$$\Gamma_1 = \frac{128\pi^2}{27} \cdot \alpha^8 \cdot \langle \delta_{+-} \rangle = 2.1315138 \cdot 10^4 \cdot \langle \delta_{+-} \rangle \ sec^{-1}, \quad (12)$$

where $\langle \delta_{+-} \rangle = \langle \delta_{++} \rangle$ in the $Ps_2$ system. By using our best-to-date numerical value for the $\langle \delta_{+-} \rangle$ expectation value ($\langle \delta_{+-} \rangle \approx 9.11034 \cdot 10^{-5}$) we can evaluate the one-photon annihilation rate in the bi-positronium $Ps_2$ as $\approx 1.94188 \cdot 10^{-1} \ sec^{-1}$. The analytical expression for the zero-photon annihilation rate in $Ps_2$ is

$$\Gamma_{0\gamma} = \frac{147\sqrt{3}\pi^3}{2} \cdot \alpha^{12} \cdot \langle \delta_{++-} \rangle = 5.0991890 \cdot 10^{-4} \cdot \langle \delta_{++-} \rangle \ sec^{-1} \quad (13)$$

where $\langle \delta_{++-} \rangle$ is the expectation value of the four-particle delta-function in the bi-positronium $Ps_2$. Now, by using the $\langle \delta_{++-} \rangle \approx 4.5614 \cdot 10^{-6}$ expectation value one finds that $\Gamma_{0\gamma}(Ps_2) \approx 2.32197 \cdot 10^{-9} \ sec^{-1}$.

Consider the cases of four- and five-photon annihilation in the bi-positronium $Ps_2$. Based on the results from [1] we can write the corresponding annihilation rates in the form

$$\Gamma_{4\gamma}(Ps_2) \approx 0.274 \left(\frac{\alpha}{\pi}\right)^2 \Gamma_{2\gamma}(Ps_2) \quad (14)$$

and

$$\Gamma_{5\gamma}(Ps_2) \approx 0.177 \left(\frac{\alpha}{\pi}\right)^2 \Gamma_{3\gamma}(Ps_2), \quad (15)$$

where $\Gamma_{4\gamma}(Ps_2)$ and $\Gamma_{5\gamma}(Ps_2)$ are the four- and five-photon annihilation rates of bi-positronium $Ps_2$. The expressions for the two- and three-photon annihilation rates are given by Eq.(10) and Eq.(11), respectively. The numerical values of these annihilation rates for the $Ps_2$ system are $\Gamma_{0\gamma} \approx 2.32197 \cdot 10^{-9} \ sec^{-1}$, $\Gamma_{1\gamma} \approx 1.94188 \cdot 10^{-1} \ sec^{-1}$, $\Gamma_{2\gamma} \approx 4.4385952 \cdot 10^9$.
\( \Gamma_3 \approx 1.202497 \cdot 10^7 \, \text{sec}^{-1} \), \( \Gamma_4 \approx 1.562 \cdot 10^9 \, \text{sec}^{-1} \), and \( \Gamma_5 \approx 11.484 \, \text{sec}^{-1} \). The \( \Gamma_4 \) and \( \Gamma_5 \) rates have not been calculated in earlier studies. The numerical computation of these annihilation rates practically solves the annihilation problem for the bi-positronium system \( \text{Ps}_2 \). A few annihilation rates, e.g., \( \Gamma_6 \) and \( \Gamma_7 \), which still remain unknown, are very small. Further, they are not of any interest in current applications. Note that in the first (and very accurate) approximation the annihilation of the \( \text{Ps}_2 \) system can be described with the use of the two annihilation rates (\( \Gamma_2 \) and \( \Gamma_3 \)) only.

IV. CONCLUSION

We have considered annihilation of the electron-positron pairs in the three-body ion \( \text{Ps}^- \) and four-body bi-positronium ‘molecule’ \( \text{Ps}_2 \). The rates of the two-, three-, four- and five-photon annihilation have been determined numerically for the ground states in each of these systems. In our calculations we have used the expectation values of delta-functions determined with the help of highly accurate wave functions. The corresponding numerical values of these annihilation rates (and also \( \Gamma_1 \) and \( \Gamma_0 \) annihilation rates) for the \( \text{Ps}^- \) ion and \( \text{Ps}_2 \) ‘molecule’ can be found in the text and Abstract. With the final computation of these annihilation rates we have to note that this work concludes many years of intense research of the problem of annihilation of electron-positron pairs from the bound (ground) states of the \( \text{Ps}^- \) ion and \( \text{Ps}_2 \) system. As follows from the results of this work, in the first (and very good) approximation annihilation in the \( \text{Ps}^- \) ion and \( \text{Ps}_2 \) system can be considered by taking into account the two largest annihilation rates only, i.e. \( \Gamma_2 \) and \( \Gamma_3 \). This conclusion can be generalized to arbitrary polyelectrons (polyleptons).

Note that the three-body \( \text{Ps}^- \) ion has been created in the laboratory by Mills [10, 11]. The total annihilation rate of the \( \text{Ps}^- \) ion has been measured in [11], where it was found that \( \Gamma (\text{Ps}^-) \approx 2.09 \cdot 10^9 \, \text{sec}^{-1} \). Annihilation rates in the bi-positronium \( \text{Ps}_2 \) have never been measured experimentally. In fact, an isolated bi-positronium ‘molecule’ \( \text{Ps}_2 \) has not been created in the laboratory. Nevertheless, the bi-positronium is of great interest in astrophysics, solid state physics and other problems (see discussion and references in [9]).

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