Title
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Positron annihilation in the bi-positronium Ps_2.

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Abstract

The $(e^-, e^+)-$pair annihilation in the bi-positronium Ps_2 (or $e^-e^+e^-e^+$) is considered. In particular, the two-, three-, one- and zero-photon annihilation rates are determined to high accuracy. The corresponding analytical expressions for these annihilation rates are also presented. By using our most recent and accurate variational wave functions produced for the ground $S(L=0)-$state of the bi-positronium Ps_2 ($E = -0.5160037754$ $a.u.$) we have found for the two-photon annihilation rate $\Gamma_{2\gamma} \approx 4.66424 \cdot 10^9$ sec^{-1}, while $\Gamma_{3\gamma}(Ps_2) \approx 1.2022 \cdot 10^6$ sec^{-1}, $\Gamma_{1\gamma} \approx 1.954 \cdot 10^{-1}$ sec^{-1} and $\Gamma_{0\gamma} \approx 2.34 \cdot 10^{-9}$ sec^{-1}. Also, a large number of bound state properties have been determined for this system.

In this study we consider the (e^-, e^+)-pair annihilation in the bi-positronium system Ps_2 (or $e^-e^+e^-e^+$). The stability of the single bound state in the bi-positronium Ps_2 has been shown many years ago [1], [2]. The bi-positronium is of great interest in some applications to astrophysics [3], solid state physics [4] and other problems [5] - [7]. Most of such applications are related to the electron-positron pair annihilation (or $(e^-, e^+)-$pair annihilation, for short) in the Ps_2 system. For instance, a long-standing problem in astrophysics is related to an unknown and very intense source of positrons in the center of our Galaxy. In fact, this source(s) is located at a distance of ≈ 8 kpc (1 $kpc \approx 3.086 \cdot 10^{16}$ km) in the direction of Galactic center with a radius ≈ 1 kpc. It generates $\approx 1.3 \cdot 10^{43}$ positrons per second [8] (or $\approx 1.18{\cdot}10^9$ tonnes of positrons per second). All these positrons annihilate in this area (so-called Galactic bulge). An intense emission of the 511 KeV annihilation $\gamma-$quanta from Galaxy bulge indicates that the (e^-, e^+)-pair annihilation proceeds mainly from the bound states of various electron-positron species (e.g., Ps, Ps^-, Ps_2, etc) and positron compounds with some atoms. Therefore, to make some quantitative evaluations one needs to know the relative probabilities of different annihilation channels in the Ps^- ion, bi-positronium Ps_2 and other similar systems.

On the other hand, the $(e^-, e^+)-$pair annihilation in the Ps_2 system is a very important problem of quantum electrodynamics. In the Ps_2 system the electron-positron annihilation proceeds with the emission of the two-, three-, ..., $n-$photons. The one- and zero-photon annihilations are also possible. Accurate evaluation of the corresponding annihilation rates is extremely complicated problem. The two-photon annihilation rate in the bi-positronium has been evaluated in [9]. Our earlier evaluations of the two-photon annihilation rate $\Gamma_{2\gamma}$ can be found in [10]. The one- and zero-photon annihilation rates in the bi-positronium have been approximately evaluated in [10].

However, in [10] we could use only very approximate variational wave functions which have relatively poor accuracy. In fact, for many two-particle bound state properties those wave functions have provided relatively good numerical accuracy. The two-particle property is an expectation value of some operator which explicitly depend upon the coordinates of the two different particles. Analogously, one can define the three- and four-particle properties in arbitrary four-body systems. As follows from the results obtained in [10] our wave functions could not provide even sufficient accuracy for a number of three- and four-particle properties in the bi-positronium Ps_2 system. In particular, the three- and four-particle delta-functions have been determined quite approximately in [10]. Furthermore, in [10] to evaluate some annihilation rates in the Ps_2 system we have used the approximate Ferrante's relations [11].

Recently, however, a remarkable progress has been achieved in obtaining the accurate variational wave functions for numerous Coulomb four-body systems. Currently, in computations of various four-body systems one can use significantly more accurate variational wave functions than the wave function used in [10]. This allow us to re-evaluate many bound state properties of the bi-positronium Ps_2. In particular, the main goal of this study is to determine the expectation values of the electron-positron delta-function $\langle \delta_{+-} \rangle$, triple delta-function $\langle \delta_{+--} \rangle = \langle \delta_{++-} \rangle$ and four-body delta-function $\langle \delta_{++--} \rangle$. These delta-functions are included in the analytical expressions for the two-, one- and zero-photon annihilation rates of the bi-positronium Ps_2. Another goal of this study was to re-derive the analytical expressions used for the two-, three-, one- and zero-photon annihilation rates. In particular, we have re-derived the corresponding analytical formulas (the formulas for one- and zero-photon annihilation rates have been originally obtained in [10] and [12]). For the two-photon annihilation rate our present formula includes the lowest-order radiative correction [13]. With the use of improved formulas and accurate expectation values for all required delta-functions this work contains the most accurate annihilation rates in the bi-positronium Ps_2 system.

The Hamiltonian of the considered Ps_2 system is written in the form (in atomic units $\hbar = 1, m_e = 1$ and $e = 1$):

$$H = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{1}{2}\Delta_3 - \frac{1}{2}\Delta_4 + \frac{1}{r_{12}} - \frac{1}{r_{13}} - \frac{1}{r_{14}} - \frac{1}{r_{23}} - \frac{1}{r_{24}} + \frac{1}{r_{34}} \qquad (1)$$

where the notation 1 and 2 designate the positrons, while 3 and 4 stand for electrons. Note that all our present calculations have been performed in atomic units ($\hbar = 1, m_e = 1$ and $e = 1$). Also, in this equation and below $r_{ij} = \mid \mathbf{r}_i - \mathbf{r}_j \mid = r_{ji}$ are the six relative coordinates uniformly defined in the considered four-body system. In fact, in all formulas and tables below, the subscripts 1 and 2 always designate the two positrons, while the subscripts 3 and 4 mean the two electrons in the bi-positronium Ps_2 ($e^- e^+ e^- e^+$). An alternative (i.e. '+' and '-') system of notation is also used below.

The corresponding Schrödinger equation is $H\Psi = E\Psi$, where E is the total bound state energy ($E < 0$) and Ψ is the bound state wave function. To determine the energies and other bound state properties of the bi-positronium Ps_2 in this study we have used the variational expansion written in the basis of six-dimensional (or four-body) gaussoids. This basis has been proposed in [14]. In fact, in [14] this variational expansion has been proposed and used for an arbitrary $N-$body non-relativistic system, but for the considered four-body systems this variational expansion takes a very simple form [14]. In particular, for the ground $S(L = 0)-$state of the Coulomb four-body Ps_2 system we have

$$\Psi(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}) = \mathcal{A}_s \sum_{i=1}^{N} C_i \Bigl[\exp(-\alpha_{12}(i) r_{12}^2 - \alpha_{13}(i) r_{13}^2 - \alpha_{23}(i) r_{23}^2 - \alpha_{14}(i) r_{14}^2 - \alpha_{24}(i) r_{24}^2 - \alpha_{34}(i) r_{34}^2)\Bigr] \quad , \tag{2}$$

where N is the total number of terms in this expansion, C_i are the linear (or variational) coefficients (here $1 \le i \le N$), while $\alpha_{kn}(i)$ ((kn) = (12), (13), (23), (14), (24) and (34)) are the non-linear parameters of the variational expansion Eq.(2). The operator $\mathcal{A}_s$ designates the appropriate symmetrizer (or antisymmetrizer), i.e. a projection operator which produces the final wave function with the correct permutation symmetry. The construction of the $\mathcal{A}_s$ is described in detail in the literature, e.g., in our earlier works [10].

In reality, the variational expansion, Eq.(2), converges very slow. Therefore, it can be effective in actual applications, if (and only if) all $6 \times N$ non-linear parameters $\alpha_{kn}(i)$ ($1 \le i \le N$ and (kn) = (12), (13), (23), (14), (24) and (34)) in Eq.(2) are carefully optimized. In this study the Powell's method of conjugate directions [15], [16] has been used. This method produces quite accurate variational wave functions for an arbitrary Coulomb four-body system. In our present calculations we have used the variational wave functions with N = 600, 700 and 800 terms. The optimization of the non-linear parameters has been produced with the use of standard double precision computer accuracy. However, to determine the expectation values of all properties we have used the extended numerical accuracy.

The obtained accurate wave function of the bi-positronium system Ps_2 allows us to determine a large number of bound state properties for this system to very good accuracy. The results of our present calculations can be found in Table I. In general, each of the properties presented in Table I is now known to much better accuracy, than it was known from our previous works (see, e.g., [10]).The observed agreement of all computed bound state properties with the numerical values presented in [17] can be considered as very good. Relatively large deviations, however, can be found (as expected) for the expectation values of the three- and four-particle delta-functions [10] which determine the one- and zero-photon annihilation rates. For instance, in Table I we have $\langle\delta_{+--}\rangle = 9.16710{\cdot}10^{-5}$ and $\langle\delta_{++--}\rangle = 4.5889{\cdot}10^{-6}$, while the best values obtained in [10] were $\langle\delta_{+--}\rangle = 9.2580{\cdot}10^{-5}$ and $\langle\delta_{++--}\rangle = 4.3908{\cdot}10^{-6}$.

As mentioned above the (e^-, e^+)-pair annihilation in the bi-positronium Ps_2 can proceed with the emission of one-, two-, three- and even larger number of photons. The zero-photon annihilation is also possible. In general, the two-photon annihilation of the (e^-, e^+)-pair has significantly larger probability than all other annihilation processes. The analytical expression for the two-photon annihilation rate which also includes the lowest-order radiative correction [18] takes the from

$$\Gamma_{2\gamma} = \pi\Big[1 - \frac{\alpha}{\pi}\Big(5 - \frac{\pi^4}{4}\Big)\Big] \cdot \alpha^4 \cdot n(ca_0^{-1}) \cdot \langle\delta_{+-}\rangle = 52.73841022 \cdot 10^9 \cdot n \cdot \langle\delta_{+-}\rangle \quad sec^{-1} \qquad (3)$$

where $\alpha \approx 0.7297352568 \cdot 10^{-2}$ is the fine structure constant, $c = 0.299792458 \cdot 10^9\ m \cdot sec^{-1}$ is the speed of light, $a_0 = 0.5291772108 \cdot 10^{-10}\ m$ is the Bohr radius. All physical constants in this study have been chosen from [19]. Also, in this equation n is the total number is the total number of electron-positron pairs, i.e. $n = 4$ in the Ps_2 system. The notation $\langle\delta_{+-}\rangle$ designates the expectation value of the electron-positron delta-function δ_{+-}. By using the expectation value for the electron-positron delta-function $\langle\delta_{+-}\rangle$ from Table I one finds that

$\Gamma_{2\gamma}(\mathrm{Ps}_2) \approx 4.664238 \cdot 10^9 \; sec^{-1}$.

The two-photon annihilation plays a leading role in the bi-positronium annihilation. The three-photon annihilation rate is $\approx$ 1000 smaller than the $\Gamma_{2\gamma}$ rate computed above, but the three-photon annihilation is of interest in a number of applications. The three-photon annihilation rate $\Gamma_{3\gamma}(\mathrm{Ps}_2)$ can be written in the form

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

By using the $\langle \delta_{+-} \rangle$ expectation value from Table I we determine that $\Gamma_{3\gamma}(\mathrm{Ps}_2) \approx 1.202155 \cdot 10^6 \; sec^{-1}$. The difference Δ between the corresponding inverse values $\frac{1}{\Gamma_{3\gamma}}$ and $\frac{1}{\Gamma_{2\gamma}}$ can be considered as the positron quenching for the bi-positronium Ps_2. The positron quenching ($\Delta \approx 8.31625 \cdot 10^{-7} \; sec$) is a unique characteristic of the considered (Ps_2) system.

The one-photon (e^-, e^+)-pair annihilation in the bi-positronium Ps_2 was considered in [10]. The one-photon annihilation rate in the Ps_2 system is written in the form

$$\Gamma_{1\gamma} = \frac{128\pi^2}{27} \cdot \alpha^8(ca_0^{-1}) \cdot \langle \delta_{+--} \rangle = 2.1315138 \cdot 10^4 \cdot \langle \delta_{+--} \rangle \quad sec^{-1} \tag{5}$$

where $\langle \delta_{+--} \rangle = \langle \delta_{++-} \rangle$ in the Ps_2 system. The one-photon annihilation is followed by the emission of one fast electron/positron. The Lorentz $\gamma-$factor of the emitted fast electron/positron is bounded between 1 and 2. By using the $\langle \delta_{+--} \rangle$ from Table I we can evaluate the one-photon annihilation rate in the bi-positronium Ps_2 as $\approx 1.95398 \cdot 10^{-1} \; sec^{-1}$.

As mentioned above the bi-positronium Ps_2 is the Coulomb four-body system. In general, the (e^-, e^+)-pair annihilation in such a system can also proceed without any emission of $\gamma-$quanta. This case corresponds to the zero-photon annihilation of the bi-positronium Ps_2. Roughly speaking, the zero-photon annihilation can be considered as the regular, two-photon annihilation of the (e^-, e^+)-pair and the following internal conversion of the two emitted $\gamma-$quanta. In reality, however, the annihilation and internal conversion of the emitted $\gamma-$quanta proceed simultaneously. The analytical expression for the zero-photon annihilation rate is

$$\Gamma_{0\gamma} = \frac{147\sqrt{3}\pi^3}{2} \cdot \alpha^{12}(ca_0^{-1}) \cdot \langle \delta_{++--} \rangle = 5.0991890 \cdot 10^{-4} \cdot \langle \delta_{++--} \rangle \quad sec^{-1} \tag{6}$$

where $\langle \delta_{++--} \rangle$ is the expectation value of the four-particle delta-function in the bi-positronium Ps_2. Now, by using our $\langle \delta_{++--} \rangle$ expectation value from Table I one finds

$$\Gamma_{0\gamma} = 2.33997 \cdot 10^{-9} \quad sec^{-1} \quad . \tag{7}$$

Thus, we have considered the annihilation of electron-positron pairs in the bi-positronium Ps_2. The closed analytical formulas and numerical values are presented for the $\Gamma_{2\gamma}, \Gamma_{3\gamma}, \Gamma_{1\gamma}$ and $\Gamma_{0\gamma}$ annihilation rates. These rates are now known to significantly better accuracy than it follows from earlier calculations. In other words, the analytical formulas and numerical values for the corresponding annihilation rates presented in this study can be considered as the final solution for the electron-positron pair annihilation in the bi-positronium system Ps_2. A large number of bound state properties of the ground state in the bi-positronium Ps_2 ($e^-e^+e^-e^+$) system have been also re-evaluated by using our recently optimized variational wave functions.

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TABLES

TABLE I. The expectation values in atomic units ($m_e = 1, \hbar = 1, e = 1$) of some properties for the ground $S(L=0)-$state of the bi-positronium Ps_2 ($e^-e^+e^-e^+$)

E	-0.51600377536	$\langle r_{++}^{-2} \rangle$	0.07344438	$\langle r_{++} \rangle$	6.0332004
$\langle T \rangle$	0.51600373242	$\langle r_{+-}^{-2} \rangle$	0.30310368	$\langle r_{+-} \rangle$	4.4871505
$\langle V \rangle$	-1.03200750796	$\langle r_{++}^{-1} \rangle$	0.22079014	$\langle r_{++}^{2} \rangle$	46.374614
χ^a	$0.4143 \cdot 10^{-7}$	$\langle r_{+-}^{-1} \rangle$	0.36839698	$\langle r_{+-}^{2} \rangle$	29.112598
$\langle r_{++}^{3} \rangle$	443.8486	$\langle r_{++}^{4} \rangle$	5201.915	$\langle -\frac{1}{2}\nabla_{+}^{2} \rangle$	0.129000933
$\langle r_{+-}^{3} \rangle$	253.0438	$\langle r_{+-}^{4} \rangle$	2807.197	$\langle -\frac{1}{2}\nabla_{-}^{2} \rangle$	0.129000933
$\langle \delta_{++} \rangle$	$6.26735 \cdot 10^{-4}$	$\langle \delta_{+--} \rangle$	$9.1671 \cdot 10^{-5}$		
$\langle \delta_{+-} \rangle$	$2.211025 \cdot 10^{-2}$	$\langle \delta_{++--} \rangle$	$4.5889 \cdot 10^{-6}$		

[a] $\chi = \mid 1 + \frac{\langle V \rangle}{2\langle T \rangle} \mid$ is the virial parameter which indicates the overall quality of the wave function used [20].