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Annihilation, bound state properties and photodetachment of the positronium negatively charged ion

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ABSTRACT

Bound state properties of the negatively charged Ps^- ion (or $e^-e^+e^-$) are discussed. The expectation values of operators which correspond to these properties have been determined with the use of the highly accurate wave functions constructed for this ion. Our best variational energy obtained for the Ps^- ion is $E = -0.2620050\ 7023298\ 0107770\ 40051$ a.u. Annihilation of the electron–positron pair(s) in the negatively charged Ps^- ion (or $e^-e^+e^-$) is considered in detail. By using accurate values for a number annihilation rates $\Gamma_{n\gamma}$, where n = 1, 2, 3, 4 and 5, we evaluated the half-life τ_a of the Ps^- ion against positron annihilation ($\tau_a = 1/\Gamma \approx 4.793584140 \times 10^{-10}$ s). Photodetachment of the Ps^- ion is considered in the long-range, asymptotic approximation. The overall accuracy of our photodetachment cross-section of the Ps^- ion is very good for such a simple approximation.

1. Introduction

The main goal of this short communication is to perform computational and theoretical analysis of the annihilation of electron-positron pair(s) in the negatively charged Ps^- ion. Another aim is to evaluate the photodetachment cross-section of the Ps^- ion in the long-range, asymptotic approximation. Our analysis is based on some recent results of highly accurate computations performed for the ground (bound) 1^1S-state in the Ps^- ion, which is also designated as the $e^-e^+e^-$ ion, or $e^+e_2^-$ ion. Stability of this three-body system was predicted by Ruark [1]. First variational calculations of the ground state in the Ps^- ion were performed by Hylleraas in 1947 [2]. This ion is of interest in various branches of physics, including solid state physics [3], astrophysics [4–6], physics of high-temperature plasmas, etc. Note that the Ps^- ion has been created experimentally by Mills almost forty years ago [7]. Review of the most recent experiments performed for the Ps^- ion can be found in [8] and [9] which also contain a large number of useful references.

As is well known from the general theory of bound states in the Coulomb three-body systems with unit charges [10] this ion has only one stable state, which is the ground 1^1S-state, or $1^1S(L=0)$-state. In general, to describe the bound 1^1S-state in this ion we can restrict ourselves to the non-relativistic *LS*-approximation, since all lowest-order relativistic and QED corrections are very small for this ion. The non-relativistic approximation means that the wave function Ψ can be determined as the solution of the non-relativistic Schrödinger equation $H\Psi = E\Psi$, where $E<0$, for three-particle quasi-atomic (or Coulomb) systems. The non-relativistic Hamiltonian H of the Ps^- ion takes the form

$$H = -\frac{\hbar^2}{2m_e}[\nabla_1^2 + \nabla_2^2 + \nabla_3^2] - \frac{e^2}{r_{31}} - \frac{e^2}{r_{32}} - \frac{e^2}{r_{21}} \quad (1)$$

where $\hbar = h/2\pi$ is the reduced Planck constant (also called Dirac constant) and m_e is the electron mass and $-e$ is the electric charge of an electron. In this equation and everywhere below in this study the subscripts 1 and 2 designate two electrons (e^-), while the subscript 3 always denotes the positron (e^+) with the mass m_e (the same electron mass) and positive electric charge $+e$, or e. In addition to the 'numerical' indexes (1, 2, 3) in some cases we shall designate electrons by using the notaiton '-', while the notation '+' always means positively charged positron. In Eq. (1) the notations $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| = r_{ji}$ stand for three interparticle distances (= relative coordinates) which are the absolute values of differences of the Cartesian coordinates $\mathbf{r}_i$ of the three particles. Note that each relative coordinate r_{ij} is a scalar which is rotationally and translationally invariant. However, these coordinates are not truly independent, since e.g., $|r_{32} - r_{31}| \le r_{21} \le r_{32} + r_{31}$. This produces a number of problems for computations of three-particle integrals in these coordinates. To simplify such calculations it is better to apply a set of three perimetric coordinates u_1, u_2, u_3 which are simply related to the relative coordinates: $u_i = \frac{1}{2}(r_{ik} + r_{jk} - r_{ij})$, while inverse relations take the form $r_{ij} = u_i + u_j$. Three perimetric coordinates u_1, u_2, u_3 are independent of each other and each of them varies between 0

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Table 1
The total energies E of the Ps^- ion (in atomic units).

K	$E(Ps^-$; variant A)	$E(Ps^-$; variant B)
3500	−0.26200507 02329801 07770398 027	−0.26200507 02329801 07770398 256
3700	−0.26200507 02329801 07770399 455	−0.26200507 02329801 07770399 614
3800	−0.26200507 02329801 07770400 032	−0.26200507 02329801 07770400 078
3840	−0.26200507 02329801 07770400 250	−0.26200507 02329801 07770400 279

and $+\infty$. The Jacobian of the transition $r_{jk} \to u_i$:$D_{u_1,u_2,u_3}(r_{32}, r_{31}, r_{21}$ is a constant which equals 2. Note also that in this study only atomic units $\hbar$=1, $|e|$=1, m_e = 1 are employed. In these units the explicit form of the Hamiltonian H, Eq. (1), is simplified to the form

$$H = -\frac{1}{2}[\nabla_1^2 + \nabla_2^2 + \nabla_3^2] - \frac{1}{r_{31}} - \frac{1}{r_{32}} + \frac{1}{r_{21}} \tag{2}$$

Note that the Hamiltonian, Eq. (2), does not contain any ratio of masses and/or electric charges. It follows from here that the Ps^- ion plays a central role in the general theory of Coulomb three-body systems with unit charges (for more details, see, e.g., [10]).

To solve the non-relativistic Schrödinger equation $H\Psi = E\Psi$ for the Ps^- ion, where $E < 0$, and obtain highly accurate wave function(s) we approximate the unknown exact solution of the non-relativistic Schrödinger equation with some efficient and fast convergent variational expansions. The best of such expansions is the exponential variational expansion in the relative coordinates r_{32}, r_{31}, r_{21}, or perimetric coordinates u_1, u_2, u_3. For the ground state of the Ps^- ion the explicit form of this expansion is

$$\begin{aligned}\Psi &= \frac{1}{2}(1 + \hat{P}_{12})\sum_{i=1}^{N} C_i \exp(-\alpha_i r_{32} - \beta_i r_{31} - \gamma_i r_{21}) \\ &= \frac{1}{2}(1 + \hat{P}_{12})\sum_{i=1}^{N} C_i \exp[-(\alpha_i + \beta_i)u_3 - (\alpha_i + \gamma_i)u_2 - (\beta_i + \gamma_i)u_3)\end{aligned} \tag{3}$$

where the notation $\hat{P}_{12}$ stands for the permutation operator of identical particles, C_i (i = 1, 2, ..., N) are the linear parameters of the exponential expansion, Eq. (3), while α_i, β_i and γ_i are the non-linear parameters of this expansion. The non-linear parameters must be varied in calculations to increase the overall efficiency and accuracy of the method. The best-to-date optimization strategy for these non-linear parameters was described in [11], while its modified version is presented in [12]. The $3N$-conditions $\alpha_i + \beta_i > 0$, $\alpha_i + \gamma_i > 0$, $\beta_i + \gamma_i > 0$ for i = 1, 2, ..., N must be obeyed to guarantee covergence of all three-particle integrlas needed in computations.

2. Expectation values

By using the highly accurate, variational wave function Ψ constructed for the ground 1^1S-state of the Ps^- ion we can determine the expectation value of an arbitrary, in principle, self-adjoint operator $\hat{X}$. This is written in the following general form

$$\langle \hat{X} \rangle = \frac{\langle \Psi \mid \hat{X} \mid \Psi \rangle}{\langle \Psi \mid \Psi \rangle} \tag{4}$$

Formally, without loss of generality below we shall assume that our wave function has a unit norm, i.e. $\langle \Psi \mid \Psi \rangle$=1 (see, discussion in [13]). The total energy is the expectation value of the Hamiltonian H, Eq. (1), i.e. $E = \langle \Psi \mid H \mid \Psi \rangle$. The total energies E of the ground 1^1S-state of the Ps^- ion determined for different trial wave functions can be found in Table 1. Other possible choices of operators $\hat{X}$ in Eq. (4) lead to the different bound state properties, or properties, for short. A number of bound state properties were determined in earlier computations of the Ps^- ion (see, e.g., [14–16] and references therein). In this study we present a large number of bound state properties of the Ps^- ion determined to very high numerical accuracy ('essentially exact'). They can be found in Table 2 (in atomic units). Physical meaning of many of these properties is clear from the notations used in Tables 1 and 2. For instance, the notation $\langle r_{ij} \rangle$ stands for the expectation value of the linear distance between particles i and j. Another notation $\langle \delta_{ij} \rangle = \langle \delta(\mathbf{r}_i - \mathbf{r}_j) \rangle$ denotes the expectation value of the (Dirac) delta-function between particles i and j, while $\langle \delta_{321} \rangle = \langle \delta(\mathbf{r}_i - \mathbf{r}_j)\delta(\mathbf{r}_i - \mathbf{r}_k) \rangle$ is the expectation value of the triple delta-function. In general, the expectation value of each delta-function is the probability to locate two (or three) particles inside of one small sphere with the radius $R \approx \Lambda_e = \alpha a_0$, where Λ_e is the Compton wavelength of electron, $\alpha = e^2/\hbar c \approx 1/137$ is the fine structure constant and a_0 is the Bohr radius (see below).

For the Ps^- ion the expectation value of the electron-positron delta-function $\langle \delta_{+-} \rangle$ determines a number of annihilation rates, including the two- and three-photon annihilation rates (see below). The expectation value of the triple delta-function $\langle \delta_{321} \rangle = \langle \delta_{+--} \rangle$ is important to predict the one-photon annihilation rate $\Gamma_{1\gamma}$. It is clear that some reliable criteria are needed to check the overall quality of the computed expectation values of delta-functions. In reality, we can introduce such criteria by considering the coincidence of the computed and predicted cusp values between each pair of particles. It was shown in early papers on Coulomb systems, including atoms and molecules [17,18], that the following expectation value:

$$\nu_{ij} = \langle \hat{\nu}_{ij} \rangle = \frac{\langle \Psi \mid \delta(\mathbf{r}_{ij}) \frac{\partial}{\partial r_{ij}} \mid \Psi \rangle}{\langle \Psi \mid \delta(\mathbf{r}_{ij}) \mid \Psi \rangle} \tag{5}$$

is always finite and its numerical value equals to $q_i q_j (m_i m_j / m_i + m_j)$, where q_i, q_j are the corresponding electrical charges of particles, while m_i, m_j are their masses. The expectation value ν_{ij} is called the cusp between two Coulomb particles i and j. The coincidence of the computed expectation value of the cusp $\nu_{ij} = \langle \hat{\nu}_{ij} \rangle$ with its expected value, i.e. with $q_i q_j (m_i m_j / m_i + m_j)$, indicates the overall quality of the expectation value of the inter-particle delta-function. In actual applications to Coulomb systems this criterion works very well. Our computed and expected cusp values are presented in Table 2. As one can see from Table 2 numerical coincidence between the predicted and computed expectation values of the electron-positron and electron-electron cusps can be considered as very good. The predicted value of the electron-positron cusp for the Ps^- ion equals $-0.5\ a.u.$, while for the electron-electron cusp one finds $0.5\ a.u.$ Unfortunately, there is no similar criterion for the triple delta-function δ_{321}, since the corresponding 'three-particle cusp' is infinte for an arbitrary Coulomb system (see, e.g., [19,20] and references therein). However, for trial functions with the finite number of regular (or non-singular) basis functions the three-particle cusp ν_{123} can be defined (this value is finite) and used in computations [20].

The notations τ_{ij} stand for the expectation values of the inter-particle cosine-functions which are defined traditionally:

$$\tau_{ij} = \langle \cos(\mathbf{r}_{ik} \hat{} \mathbf{r}_{jk}) \rangle = \langle \frac{\mathbf{r}_{ik}}{r_{ik}} \cdot \frac{\mathbf{r}_{jk}}{r_{jk}} \rangle \tag{6}$$