Positron annihilation in the positronium negative ion

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Positron annihilation in the positronium negative ion

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Abstract. A theoretical study of positronium negative ions is carried out in this paper. Hylleraas-type wavefunctions are employed to describe the system and an improved ground-state energy is reported. In addition, the two-photon annihilation rate and the lifetime against two-photon annihilation are also calculated, as well as the two-photon angular correlation function.

1. Introduction

A positronium negative ion (Ps^-) is a bound three-particle system consisting of two electrons and one positron which interact via Coulomb forces. The calculation of the binding energy of this system has a long history (see Ho 1979) that can be traced back to the early work of Wheeler (1946). Recently this system has been observed for the first time in the laboratory by Mills (1981a). The production of these positronium negative ions opens up many possible research areas for experimentalists for some years to come, and in turn may stimulate more theoretical investigations. In many aspects the positronium negative ions have properties similar to those of hydrogen negative ions, H^-, a system which has been intensively studied by both theorists and experimentalists. For example, these two systems both have only one bound state, and some S-wave autoionising states in Ps^- have been predicted by Ho (1979), and can be shown, by changing the mass of the positively charged particles, to be in one to one correspondence to the known H^- counterparts. The question of the existence of a $2p^2\,{}^3P^e$ metastable state in Ps^- has been investigated by Mills (1981b) and by Bhatia and Drachman (1981).

In many respects these two systems differ only in the mass of the positively charged particles. There are, however, many properties which are unique in Ps^- and have no counterparts in H^-. These properties involve the annihilation of the positrons in the positronium negative ions. Since the positron will annihilate with one of the two electrons, the lifetime and the two-photon annihilation rate are of obvious interest. Other areas of interest are the two-photon angular correlation function; three- and one-photon annihilation rates, etc, to name just a few. On the practical side the use of positrons to study properties of solids has been proven to be a useful tool, and the research on positronium chemistry has begun to attract more attention in recent years (see a review by Schrader 1979). In astrophysical applications positronium annihilation has been observed in solar flares (Crannell *et al* 1976); in the centre of our galaxy, the Milky Way (Leventhal *et al* 1978); and in gamma ray bursts (Cline 1980). (Also see reviews by Drachman 1982 and Massey 1982.) The role that the positronium

negative ions play in astrophysics and space physics has been suggested by Sivaram and Krishan (1982). Another interesting theoretical aspect of the positronium negative ion is that it is a three-body atomic system. Historically, a three-body system represents the simplest non-trivial problem that has fascinated theorists for years in different branches of physics. In atomic physics one of the latest theoretical discoveries is the underlying symmetry of the doubly excited resonances in H^- and in helium. The striking similarity between the doubly excited spectrum of a two-electron atom and that of a linear triatomic molecule (XYX) have been investigated by Kellman and Herrick (1980). In positronium negative ions, the study of the doubly excited resonances has just begun (Ho 1979). Whether such highly symmetrical spectra will also be found in Ps^- is an open and interesting question.

In this work we have carried out a study of the ground $^1S^e$ state of Ps^-. We will report a variational energy which has the lowest value in the literature to date. In addition, once the wavefunctions have been obtained, they will be applied to calculate the two-photon annihilation rate and the lifetime of Ps^-. Furthermore, the two-photon angular correlation function will also be calculated.

2. Hamiltonian and wavefunctions

The Hamiltonian of the positronium negative ion is

$$H = T + V \tag{1}$$

where T and V are the kinetic energy and potential energy operators, respectively, and

$$T = -\frac{1}{m_1}\nabla_1^2 - \frac{1}{m_2}\nabla_2^2 - \frac{1}{m_p}\nabla_p^2 \tag{2}$$

$$V = -\frac{2}{r_{1p}} - \frac{2}{r_{2p}} + \frac{2}{r_{12}} \tag{3}$$

where 1, 2 and p denote the electrons 1, 2 and the positron respectively. The mass for particle i is m_i; and r_{ij} represents the distance between particles i and j. Atomic units are used in this work, with energy expressed in rydbergs. Hylleraas-type wavefunctions of the form

$$\Psi = \sum_{\substack{l \geqslant m \geqslant 0 \\ k \geqslant 0}} C_{klm} \exp[-\alpha(r_{1p} + r_{2p})] r_{12}^k (r_{1p}^l r_{2p}^m + r_{1p}^m r_{2p}^l) \tag{4}$$

are employed to represent the system, where $(k + l + m) \leqslant \omega$, where ω is a positive integer. The calculation can be simplified by expressing the kinetic operator in terms of distance coordinates, and equation (2) becomes

$$\begin{aligned} T = &-\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\left(\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right) - \left(\frac{1}{m_1} + \frac{1}{m_p}\right)\left(\frac{\partial^2}{\partial r_{1p}^2} + \frac{2}{r_{1p}}\frac{\partial}{\partial r_{1p}}\right) \\ &-\left(\frac{1}{m_2} + \frac{1}{m_p}\right)\left(\frac{\partial^2}{\partial r_{2p}^2} + \frac{2}{r_{2p}}\frac{\partial}{\partial r_{2p}}\right) - \frac{1}{m_1}\cos(\theta_{12,1p})\frac{\partial^2}{\partial r_{12}\,\partial r_{1p}} \\ &-\frac{1}{m_2}\cos(\theta_{12,2p})\frac{\partial^2}{\partial r_{12}\,\partial r_{2p}} - \frac{1}{m_p}\cos(\theta_{1p,2p})\frac{\partial^2}{\partial r_{1p}\,\partial r_{2p}} \end{aligned} \tag{5a}$$

with

$$\cos(\theta_{1p,2p}) = (r_{1p}^2 + r_{2p}^2 - r_{12}^2)/2r_{1p}r_{2p}, \text{ etc.} \tag{5b}$$

3. Results and discussions

Up to $N = 125$ terms ($\omega = 9$) are used in this work. The ground-state energy is optimised for a given ω, with ω having values of $\omega = 3$, 4, 5, 6, 7, 8, and 9, which correspond to $N = 13$, 22, 34, 50, 70, 95, and 125 respectively. Results are reported in table 1 together with the optimised non-linear parameter α of the wavefunction. The energy of $E = -0.524\,009\,79$ Ryd, obtained by the use of a 125 term wavefunction, represents the lowest energy of Ps^- in the literature to date. To test the qualities of the wavefunctions, we have calculated the electron–electron and electron–positron cusp values. For a system interacting through Coulomb forces, the average value of the cusp condition between particles i and j is given by (Chong and Schrader 1969)

$$\nu_{ij} = \left\langle \Psi \middle| \delta(r_{ij}) \frac{\partial}{\partial r_{ij}} \middle| \Psi \right\rangle (\langle \Psi | \delta(r_{ij}) | \Psi \rangle)^{-1} \tag{6}$$

and the exact value for ν_{ij} is

$$\nu_{ij} = q_i q_j \mu_{ij} \tag{7}$$

where q_i is the charge for the particle i and μ_{ij} is the reduced mass for particles i and j. The exact values for electron–electron and electron–positron conditions are hence $+0.5$ and -0.5 respectively. The cusp values calculated by using the energy minimised wavefunctions are shown in table 1. It is seen that the cusp results are very close to the exact values. These cusp results are consistent with those obtained by Bhatia and Drachman (1982). The results shown in table 1 also demonstrate the lack of any bound theorem for the cusp values.

One of the experimentally interesting parameters is the two-photon annihilation rate, Γ, given in units of ns^{-1} (see Fraser 1968, for example)

$$\Gamma = 50.47n \frac{\langle \Psi | \delta(r_1 - r_p) | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{8}$$

where n is the number of electrons in the system. In the present case, of course, n has a value of two. The lifetime of Ps^- against two-photon annihilation is

$$\tau = 1/\Gamma. \tag{9}$$

Again, once the energy-minimised wavefunctions are obtained, they can be used to calculate Γ by the use of equation (8). The results are shown in table 1. It is seen that the results for Γ are quite stable when the wavefunctions are sufficiently large. It also demonstrates the lack of a bound property for Γ. With the 125 term wavefunction, we obtain a value for the two-photon annihilation rate

$$\Gamma = 2.0908\ ns^{-1}.$$

This corresponds to a lifetime against two-photon annihilation of

$$\tau = 0.478\ ns.$$

Table 1. Annihilation rates, two-photon angular correlations, and other atomic properties for positronium negative ions.

N	α	$-E$ (Ryd)	2Δ (mrad)	Γ (ns^{-1})	ν_{1P} (a_0^{-1})	ν_{12} (a_0^{-1})	$\langle r_{1P} \rangle$ (a_0)	$\langle r_{1P}^2 \rangle$ (a_0^2)	$\langle r_{1P}^{-1} \rangle$ (a_0^{-1})	$\langle r_{12} \rangle$ (a_0)	$\langle r_{12}^2 \rangle$ (a_0^2)	$\langle r_{12}^{-1} \rangle$ (a_0^{-1})
13	0.3620	0.522 013 72	1.7906	1.9617	−0.4681	0.4813	5.1143	38.8305	0.3429	7.8423	74.8089	0.1637
22	0.3410	0.523 886 26	1.4879	2.0723	−0.4928	0.5110	5.4290	44.4408	0.3402	8.4320	89.3219	0.1565
34	0.3490	0.523 915 17	1.4903	2.0688	−0.4912	0.5101	5.4325	46.5284	0.3402	8.4386	89.4643	0.1565
50	0.3450	0.524 001 81	1.4184	2.0890	−0.4982	0.5068	5.4799	48.0367	0.3399	8.5295	92.4264	0.1557
70	0.3365	0.524 005 53	1.4110	2.0870	−0.4973	0.5013	5.4848	48.2180	0.3398	8.5392	92.7801	0.1557
95	0.3475	0.524 009 34	1.4006	2.0911	−0.4993	0.4987	5.4886	48.3700	0.3398	8.5465	93.0819	0.1556
125	0.3560	0.524 009 79	1.3994	2.0908	−0.4991	0.4971	5.4891	48.3936	0.3398	8.5476	93.1283	0.1556

It is seen that the results obtained in this paper are very close to the spin average annihilation rate and lifetime for a positronium atom. An explanation was provided by Drachman (1982); since a positronium negative ion is a loosely bound system (a positronium atom plus something), annihilations will mostly involve the electron in the positronium atom. Even very elaborate wavefunctions, such as those employed in the present calculation, improve the results by only a small amount. It should also be mentioned that Ferrante (1968), with a six-parameter wavefunction, obtained results for the Γ and τ values of $1.99\ \text{ns}^{-1}$ and 0.502 ns respectively. The present results hence represent an improvement of about 5% over previous data in the literature.

In addition to the lifetimes and annihilation rates, another experimentally interesting parameter for the positronium negative ion is the two-photon angular correlation function $P(\theta)$. In most of the angular correlation measurements only one component of the momentum distribution is measured. The angle between the two photons, measured in the laboratory frame, has a value of $\pi - \theta$. The relation between θ and q_3, the third component of the momentum, is $q_3 = mc\theta$, or $\theta = 7.3 \times 10^{-3} q_3$. The one-dimensional angular correlation function will have a form (see Drachman and Temkin 1972 and Humberston and Wallace 1972, for example)

$$P(q_3) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}q_1\, \mathrm{d}q_2\, S(\boldsymbol{q}) \tag{10}$$

where

$$S(\bar{q}) = \left| \int \mathrm{d}\boldsymbol{r}_{1p} \exp(-\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}_{1p}) \Psi(\boldsymbol{r}_{1p}, \boldsymbol{r}_{2p}, \boldsymbol{r}_{12})_{\substack{r_{12}=r_{1p} \\ r_{2p}=0}} \right|^2. \tag{11}$$

The final results for the angular correlation function are obtained by using the 125 term wavefunction and are plotted in figure 1, with the maximum normalised to unity. The full width at the half maximum, denoted by 2Δ, is 1.3994×10^{-3} rad. This represents a factor of approximately six smaller than the counterpart in, say, e^+–He zero-energy scattering (Humberston 1979). (A positron does not bind to the ground state of a helium atom.) Other values of 2Δ for smaller expansion lengths are also shown in table 1. The smaller width of the angular correlation function for Ps^- is due to the following. Since the Ps^- ion is a loosely bound system, the momentum distribution of the Ps atom in Ps^- is smaller than the more tightly bound atomic counterparts. The angular correlation function for Ps^- is hence smaller. Furthermore, when the positron annihilates with one of the electrons in Ps^- to become two photons, a portion of the momentum of the two photons will be absorbed by the remaining electron because the mass of the electron is small. This would also contribute to the small width for the angular correlation function. It should be mentioned that the two-photon angular correlation function was claimed to be calculated by Ferrante (1968). However, the result obtained by Ferrante was not the one-dimensional angular correlation function. Therefore, no comparison with the present findings is possible.

In table 1, we also report the average distance between the two electrons $\langle r_{12} \rangle$ and between the positron and an electron $\langle r_{1p} \rangle$ etc. The results for these parameters calculated by the 125 term wavefunction are 8.5476 and 5.4891 a_0 for $\langle r_{12} \rangle$ and $\langle r_{1p} \rangle$ respectively. These results do indicate that in order to form such an ion, a large free space is required. The present findings are qualitatively consistent with those obtained by Ferrante (1968) with a simpler wavefunction.

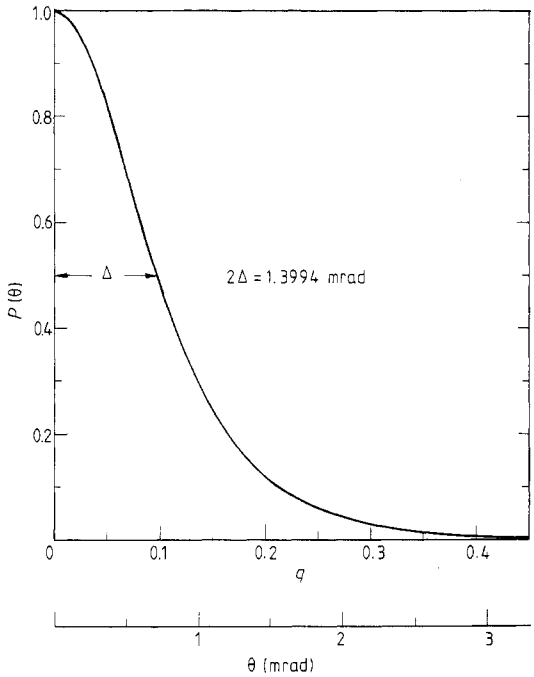

Figure 1. Two-photon angular correlation function in the positronium negative ions.

In summary we have carried out a calculation of some parameters for the positronium negative ion. These include the ground-state energy, the two-photon annihilation rate and lifetime, as well as the two-photon angular correlation. The results reported in this work are believed to be quite accurate, and should be useful for future experimental references.

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Note added in proof. Some recent developments in the studies of Ps^- ions have been brought to my attention. From the experimental side, A P Mills Jr has determined, for the first time in the laboratory, the total decay rate of Ps^-. His value of $\Gamma = 2.09 \pm 0.09\ ns^{-1}$ agrees favourably with the present two-photon calculation of $2.0908\ ns^{-1}$. From the theoretical side, A K Bhatia and R J Drachman have obtained the ground-state energy and two-photon annihilation rate of $-0.524\ 010\ 112\ 7$ Ryd and $2.0928\ ns^{-1}$, respectively, by the use of a 220 term Hylleraas-type wavefunction.

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