Calculation of density matrices in the formation of positronium

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We study single collisions between spin-polarized positron beams and targets that result in the production of positronium and target ions. We consider unpolarized as well as polarized targets with 0, 1, and 2 unpaired electrons. First, we use angular momentum coupling to calculate the spin scattering matrices in all three cases. Then, for some targets, we define an angle β between the polarization vectors of the positron beam and the target, and calculate density matrices whose elements are functions of β. Finally, from the density matrices, we obtain the probabilities of forming para- and ortho-positronium atoms for specific spins of the target ions. We present ratios of para- to ortho-positronium yields as well as total positronium annihilation rates.

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I. INTRODUCTION

In this work, we study collisions between spin-polarized positrons and atomic or molecular targets in each of which only two outgoing species are produced, a positronium atom and a target ion. The initial system consists of a purely electronic part (the target) interacting with a part containing no electrons (the positron beam). Specifically, we consider the collision of the positron beam from three types of targets: (i) a singlet with no unpaired electrons and a total unpaired-electron spin of 0, (ii) a doublet with one unpaired electron and a total unpaired-electron spin of $\frac{1}{2}$, and (iii) a triplet, with two unpaired electrons and a total unpaired-electron spin of 1. During the interaction, one electron from the target combines with the positron to form positronium. Both *para*-positronium, with a total spin of 0, and *ortho*-positronium, with a total spin of 1, are produced along with target ions with spins of 0, $\frac{1}{2}$, 1, or $\frac{3}{2}$. With the assumption that spin-dependent interaction terms in the Hamiltonian are negligible, the total spin of the unpaired electron(s) of the target, the spin of the positron, the total spin of the electron(s)-positron system, and the total spin magnetic quantum number are conserved. First, we use angular momentum coupling techniques to calculate the spin scattering matrices for each of the three types of targets. Then, we construct spin density matrices for describing the initial (positron-target) systems as well as the final (positronium-ion) systems, which consist of mixed-spin states. Density matrices are particularly useful in the description of systems containing mixed-spin states because their elements can be used to obtain the probability of the system being in a specific spin state. We construct the spin density matrices from Pauli spin matrices, and polarization vectors and tensors, using techniques described in Refs. [1–3].

Positrons obtained from a nuclear decay are longitudinally polarized with speeds close to that of the speed of light, while the energy of the positron beam used in the collisions is a few electron volts. In the laboratory frame, the polarization vector of an electrostatically guided beam remains constant, although the propagation direction given by the momentum vector can be changed. The degree to which the positron spin is aligned with the initial momentum is given by the polarization p_p. Slow polarized positron beams with values of p_p ranging from 0.5 to 0.8 have been available for some time [4]. In our work, we define an angle β between the polarization vectors of the positron beam and the target, such that, for positrons with polarization p_p, the components of the positron beam parallel and perpendicular to the direction of the target polarization vector are given by $p_p\cos\beta$ and $p_p\sin\beta$. We note (i) that $\beta = 0$ for the singlet, (ii) that for an unpolarized target, when the spin of the outgoing target ion is detected, β is the angle between the polarization vector of the positron beam and the axis of the spin detector, and (iii) that β cannot be defined for unpolarized targets *without* detection of the spin of the outgoing ion. The elements of the spin density matrices will therefore contain functions of β and p_p.

From the spin density matrices, we calculate the probabilities for forming both types of positronium, just after the collision at time $t = 0$, for specific spins of the target ions. The two types of positronium are distinguished by their lifetimes and the number of photons emitted when they decay; para-positronium decays with the emission of two photons and has a lifetime of $\frac{1}{8}$ ns [5] while ortho-positronium decays with the emission of three photons and has a lifetime of 142 ns [6–8]. We present three types of results: (i) the total positronium annihilation rates at $t = 0$, (ii) the ratios of para-to ortho-positronium yields at $t = 0$, and (iii) para-positronium and ortho-positronium yields as functions of time. We consider unpolarized as well as polarized targets and look at special cases for which $\beta = 0^\circ$, 90°, or 180°.

We introduced β in an earlier work and used angular momentum coupling as well as density-matrix techniques to study positronium formation in the collisions of polarized positron beams with molecular oxygen targets [9]. Molecular oxygen is an example of a triplet, and therefore the density-matrix equations given in Ref. [9] are identical to those for the triplet case presented in this work. However, in the present study, we have calculated the scattering matrices using Racah coefficients, as shown in the following. This enables us to present a more general formalism with several possibilities of the target spin (whereas in Ref. [9], the scattering matrices were calculated using Clebsch-Gordan coefficients only for a target spin of 1). Furthermore, in this work, we have explained our method in more detail and extended it to include singlet targets, as well as unpolarized doublet and polarized doublet targets. Since the degree of polarization p_p is controlled by the experimenter, we have presented our results for arbitrary values of p_p. We have also calculated annihilation rates and yields for all the targets for $p_p = 0.5$ (whereas in Ref. [9], the ratios of the para-positronium to ortho-positronium yields

were calculated only for $p_p = 1$), as well as additional results for a triplet target.

In our method, described in the following, we obtain scattering-matrix elements from vector coupling coefficients using techniques similar to those in Refs. [3,10,11], in which numerous results are presented for elastic scattering, excitation, and ionization processes involving polarized electrons [10,11]. We construct density matrices using formalism similar to Refs. [3,12,13] for positron collisions with targets of spin 0, $\frac{1}{2}$, and 1. In Ref. [12], the excitation of light atoms such as sodium and lithium as well as heavier atoms such as mercury due to impact with unpolarized or polarized electrons is studied. Explicit spin-dependent forces are neglected in the study of collisions with light atoms, while reduced density matrices of the scattered electrons are constructed to get polarization information for heavier atoms [12]. In Ref. [13], the effect of beam polarization on the scattering cross section is discussed in general, and scattering matrices and density matrices are calculated in the scattering of an electron by targets of spin $\frac{1}{2}$ and spin 1. In Ref. [14], the effect of spin dependence is studied in the scattering of polarized electrons by two-electron atoms. Ratios of the scattered to incident beam polarizations are compared for processes in which explicit spin-dependent forces can be neglected (electron exchange in the excitation of helium) and those in which spin-dependent forces cannot be neglected (electron-spin reversal in the excitation of mercury) [14]. The role of polarization in nuclear scattering and reaction processes has been extensively studied in Ref. [15]. Calculations of cross sections, density matrices, and polarization components of particles are performed for processes in which the polarizations of one or both particles in the initial or final states are known [15]. Since we assume that spin-dependent forces are negligible, our method may not be applicable in the study of heavy atoms or in determining left-right asymmetries in the cross section as discussed in Refs. [13–15]. We impose the conservation of four spin quantum numbers and calculate the probabilities of both outgoing particles (positronium atom and target ion) being in a specific spin state.

II. METHOD

In this section we describe the general framework for the construction of the spin density matrices for the outgoing ion-positronium system ρ_{out} from the spin density matrices for the incoming target-positron system ρ_{in} and the spin scattering matrices $\mathbf{M}$ as follows:

$$\rho_{\text{out}} = \mathbf{M}\rho_{\text{in}}\mathbf{M}^{\dagger}. \tag{1}$$

We express the three reactions under consideration as $e + p \rightarrow i + d$, where e represents the target with 0, 1, or 2 unpaired electrons, p represents the positron, i represents the target ion with one unpaired electron less than the target, and d represents both types of positronium. We begin by constructing the spin scattering matrices whose matrix elements are the amplitudes for the transition from a particular state of e and p to a particular state of i and d. As the two initial species e and p approach and interact, an intermediate state develops in which particle transfer can occur. After the particle transfer has taken place, the intermediate state decays into the outgoing species i and d which recede from the interaction site. It is important to note that in the evolution of the system from e and p to i and d, the quantum numbers representing the total electron spin S_e of the atomic target, the positron spin S_p, the total spin S_t, as well as the magnetic quantum numbers M_t are all conserved. With the assumption of a spin-independent Hamiltonian where states with different values of S_e can have different interelectronic Coulomb interactions via the Pauli principle, we define a scattering amplitude f^{S_e} which is independent of S_p, S_t, and M_t as follows:

$$f^{S_e} = \langle [S_e S_p] S_t M_t | \hat{M} | [S_e S_p] S_t M_t \rangle . \tag{2}$$

The coupled state $\langle [S_e S_p] S_t M_t |$ can be obtained from coupling the quantum numbers S_e and S_p through Clebsch-Gordan coefficients. Keeping this in mind, we express the spin scattering matrix in terms of the scattering amplitude and the intermediate state as follows:

$$\begin{aligned} &\langle S_i M_i | \langle S_d M_d | \hat{M} | S_e M_e \rangle | S_p M_p \rangle \\ &\quad = \langle S_i M_i | \langle S_d M_d | \sum_{S_t M_t} | [S_e S_p] S_t M_t \rangle f^{S_e} \\ &\qquad \times \langle [S_e S_p] S_t M_t | | S_e M_e \rangle | S_p M_p \rangle . \end{aligned} \tag{3}$$

The rows represent the final states of the target ion and positronium, while the columns represent the initial states of the target and the positron. The states are labeled with the spin and magnetic quantum numbers in each case.

First, the states of the incoming species are coupled as follows:

$$|S_e M_e\rangle |S_p M_p\rangle = \sum_{S_t M_t} \langle S_e M_e S_p M_p | S_t M_t \rangle | [S_e S_p] S_t M_t \rangle . \tag{4}$$

Then, after particle transfer has occurred, the intermediate state evolves into a coupled state of the outgoing species i and d. This relation is obtained by the U coefficients as follows:

$$|[S_e S_p] S_t M_t\rangle = \sum_{S_d} U \left(S_i \frac{1}{2} S_t S_p ; S_e S_d \right) |[S_i S_d] S_t M_t\rangle . \tag{5}$$

We note that the U coefficients of Jahn are related to the standard Racah coefficients through $U = \sqrt{(2S_e + 1)(2S_d + 1)}W$, where W is the standard Racah coefficient [16]. Finally, the outgoing state is uncoupled as follows:

$$|[S_i S_d] S_t M_t\rangle = \sum_{M_i M_d} \langle S_i M_i S_d M_d | S_t M_t \rangle | S_i M_i \rangle | S_d M_d \rangle . \tag{6}$$

When the positron beam collides with a singlet, the spin assignments for the particles are $S_e = 0$, $S_p = \frac{1}{2}$, $S_i = \frac{1}{2}$, and $S_d = 0$, 1. In the collision with a doublet with $S_e = \frac{1}{2}$, the outgoing target ion can be in the $S_i = 0$ or in the $S_i = 1$ state, whereas for the triplet target with spin $S_e = 1$, the outgoing target ion can be in the $S_i = \frac{1}{2}$ or in the $S_i = \frac{3}{2}$ state. We use these spin assignments along with all the possible magnetic quantum numbers M_e, M_p, M_i, and M_d in Eqs. (3)–(6) to obtain the spin scattering matrices $\langle S_i M_i | \langle S_d M_d | \hat{M} | S_e M_e \rangle | S_p M_p \rangle$, shown in Table I, for all three types of targets.

We now write down the individual spin density matrices for each of the three targets as well as the positron beam, using techniques from Ref. [3], after defining ε_1 and ε_2 as unit matrices of rank 2, E_1 as a unit matrix of rank 3, σ_x and σ_z as Pauli spin matrices, S_x, S_y, and S_z as spin matrices of rank 3,

TABLE I. Spin scattering matrices $\langle S_i M_i | \langle S_d M_d | \hat{M} | S_e M_e \rangle | S_p M_p \rangle$ for the reactions $e + p \rightarrow i + d$. The columns are labeled with the initial-state basis vectors $|S_e M_e\rangle|S_p M_p\rangle$, where e represents a singlet with $S_e = 0$, a doublet with $S_e = \frac{1}{2}$, or a triplet with $S_e = 1$, and p represents the positron with $S_p = \frac{1}{2}$. The rows are labeled with the final-state basis vectors $\langle S_i M_i | \langle S_d M_d |$, where i represents the singlet ion with $S_i = \frac{1}{2}$, the doublet ion with $S_i = 0$ or $S_i = 1$, or the triplet ion with $S_i = \frac{1}{2}$ or $S_i = \frac{3}{2}$, and d represents positronium.

Singlet	$\|00\rangle\|\frac{1}{2}\frac{1}{2}\rangle$	$\|00\rangle\|\frac{1}{2}-\frac{1}{2}\rangle$				
$\langle\frac{1}{2}\frac{1}{2}\|\langle 00\|$	$-\frac{1}{2}f^0$					
$\langle\frac{1}{2}-\frac{1}{2}\|\langle 00\|$		$-\frac{1}{2}f^0$				
$\langle\frac{1}{2}\frac{1}{2}\|\langle 10\|$	$\frac{1}{2}f^0$					
$\langle\frac{1}{2}\frac{1}{2}\|\langle 1-1\|$		$\sqrt{\frac{1}{2}}f^0$				
$\langle\frac{1}{2}-\frac{1}{2}\|\langle 11\|$	$-\sqrt{\frac{1}{2}}f^0$					
$\langle\frac{1}{2}-\frac{1}{2}\|\langle 10\|$		$-\frac{1}{2}f^0$				
Doublet	$\|\frac{1}{2}\frac{1}{2}\rangle\|\frac{1}{2}\frac{1}{2}\rangle$	$\|\frac{1}{2}\frac{1}{2}\rangle\|\frac{1}{2}-\frac{1}{2}\rangle$	$\|\frac{1}{2}-\frac{1}{2}\rangle\|\frac{1}{2}\frac{1}{2}\rangle$	$\|\frac{1}{2}-\frac{1}{2}\rangle\|\frac{1}{2}-\frac{1}{2}\rangle$		
$\langle 00\|\langle 00\|$		$\sqrt{\frac{1}{2}}f^{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}f^{\frac{1}{2}}$			
$\langle 00\|\langle 11\|$	$f^{\frac{1}{2}}$					
$\langle 00\|\langle 10\|$		$\sqrt{\frac{1}{2}}f^{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}f^{\frac{1}{2}}$			
$\langle 00\|\langle 1-1\|$				$f^{\frac{1}{2}}$		
$\langle 11\|\langle 00\|$	$-\sqrt{\frac{1}{3}}f^{\frac{1}{2}}$					
$\langle 10\|\langle 00\|$		$-\sqrt{\frac{1}{6}}f^{\frac{1}{2}}$	$-\sqrt{\frac{1}{6}}f^{\frac{1}{2}}$			
$\langle 1-1\|\langle 00\|$				$-\sqrt{\frac{1}{3}}f^{\frac{1}{2}}$		
$\langle 11\|\langle 10\|$	$\sqrt{\frac{1}{3}}f^{\frac{1}{2}}$					
$\langle 11\|\langle 1-1\|$		$\sqrt{\frac{2}{3}}f^{\frac{1}{2}}$				
$\langle 10\|\langle 11\|$	$-\sqrt{\frac{1}{3}}f^{\frac{1}{2}}$					
$\langle 10\|\langle 10\|$		$-\sqrt{\frac{1}{6}}f^{\frac{1}{2}}$	$\sqrt{\frac{1}{6}}f^{\frac{1}{2}}$			
$\langle 10\|\langle 1-1\|$				$\sqrt{\frac{1}{3}}f^{\frac{1}{2}}$		
$\langle 1-1\|\langle 11\|$			$-\sqrt{\frac{2}{3}}f^{\frac{1}{2}}$			
$\langle 1-1\|\langle 10\|$				$-\sqrt{\frac{1}{3}}f^{\frac{1}{2}}$		
Triplet	$\|11\rangle\|\frac{1}{2}\frac{1}{2}\rangle$	$\|11\rangle\|\frac{1}{2}-\frac{1}{2}\rangle$	$\|10\rangle\|\frac{1}{2}\frac{1}{2}\rangle$	$\|10\rangle\|\frac{1}{2}-\frac{1}{2}\rangle$	$\|1-1\rangle\|\frac{1}{2}\frac{1}{2}\rangle$	$\|1-1\rangle\|\frac{1}{2}-\frac{1}{2}\rangle$
$\langle\frac{1}{2}\frac{1}{2}\|\langle 00\|$		$\sqrt{\frac{1}{2}}f^1$	$-\frac{1}{2}f^1$			
$\langle\frac{1}{2}-\frac{1}{2}\|\langle 00\|$				$\frac{1}{2}f^1$	$-\sqrt{\frac{1}{2}}f^1$	
$\langle\frac{1}{2}\frac{1}{2}\|\langle 11\|$	f^1					
$\langle\frac{1}{2}\frac{1}{2}\|\langle 10\|$		$\sqrt{\frac{1}{2}}f^1$	$\frac{1}{2}f^1$			
$\langle\frac{1}{2}\frac{1}{2}\|\langle 1-1\|$				$\sqrt{\frac{1}{2}}f^1$		
$\langle\frac{1}{2}-\frac{1}{2}\|\langle 11\|$			$\sqrt{\frac{1}{2}}f^1$			
$\langle\frac{1}{2}-\frac{1}{2}\|\langle 10\|$				$\frac{1}{2}f^1$	$\sqrt{\frac{1}{2}}f^1$	
$\langle\frac{1}{2}-\frac{1}{2}\|\langle 1-1\|$						f^1
$\langle\frac{3}{2}\frac{3}{2}\|\langle 00\|$	$-\sqrt{\frac{3}{8}}f^1$					
$\langle\frac{3}{2}\frac{1}{2}\|\langle 00\|$		$-\sqrt{\frac{1}{8}}f^1$	$-\frac{1}{2}f^1$			
$\langle\frac{3}{2}-\frac{1}{2}\|\langle 00\|$				$-\frac{1}{2}f^1$	$-\sqrt{\frac{1}{8}}f^1$	
$\langle\frac{3}{2}-\frac{3}{2}\|\langle 00\|$						$-\sqrt{\frac{3}{8}}f^1$
$\langle\frac{3}{2}\frac{3}{2}\|\langle 10\|$	$\sqrt{\frac{3}{8}}f^1$					

TABLE I. (*Continued.*)

Triplet	$\|11\rangle\|\frac{1}{2}\frac{1}{2}\rangle$	$\|11\rangle\|\frac{1}{2}-\frac{1}{2}\rangle$	$\|10\rangle\|\frac{1}{2}\frac{1}{2}\rangle$	$\|10\rangle\|\frac{1}{2}-\frac{1}{2}\rangle$	$\|1-1\rangle\|\frac{1}{2}\frac{1}{2}\rangle$	$\|1-1\rangle\|\frac{1}{2}-\frac{1}{2}\rangle$
$\langle\frac{3}{2}\frac{3}{2}\|\langle 1-1\|$		$\sqrt{\frac{3}{4}}f^1$				
$\langle\frac{3}{2}\frac{1}{2}\|\langle 11\|$	$-\frac{1}{2}f^1$					
$\langle\frac{3}{2}\frac{1}{2}\|\langle 10\|$		$-\sqrt{\frac{1}{8}}f^1$	$\frac{1}{2}f^1$			
$\langle\frac{3}{2}\frac{1}{2}\|\langle 1-1\|$				$\sqrt{\frac{1}{2}}f^1$		
$\langle\frac{3}{2}-\frac{1}{2}\|\langle 11\|$			$-\sqrt{\frac{1}{2}}f^1$			
$\langle\frac{3}{2}-\frac{1}{2}\|\langle 10\|$				$-\frac{1}{2}f^1$	$\sqrt{\frac{1}{8}}f^1$	
$\langle\frac{3}{2}-\frac{1}{2}\|\langle 1-1\|$						$\frac{1}{2}f^1$
$\langle\frac{3}{2}-\frac{3}{2}\|\langle 11\|$					$-\sqrt{\frac{3}{4}}f^1$	
$\langle\frac{3}{2}-\frac{3}{2}\|\langle 10\|$						$-\sqrt{\frac{3}{8}}f^1$

and setting $S_{zz}=3S_z^2-\vec{S}\cdot\vec{S}$. The simplest case is for the singlet with

$$\rho_{\rm in}=1. \tag{7}$$

For the doublet with a pure z component of polarization,

$$\rho_{\rm in}=\tfrac{1}{2}(\varepsilon_1+P_z\sigma_z), \tag{8}$$

with $P_z=\mathrm{tr}(\rho_{\rm in}\ \sigma_z)=\pm 1$, while for an unpolarized target $P_z=0$. For the triplet with pure z components for both vector and tensor polarizations,

$$\rho_{\rm in}=\tfrac{1}{3}\big(E_1+\tfrac{3}{2}P_zS_z+\tfrac{1}{2}P_{zz}S_{zz}\big), \tag{9}$$

with $P_z=\mathrm{tr}(\rho_{\rm in}S_z)$ and $P_{zz}=\mathrm{tr}(\rho_{\rm in}S_{zz})$. For $P_z=\pm 1$, $P_{zz}=1$, for $P_z=0$, $P_{zz}=-2$, and for the unpolarized target $P_z=P_{zz}=0$. For the positron with polarization p_p

$$\rho_{\rm in}=\tfrac{1}{2}(\varepsilon_2+p_p\cos\beta\sigma_z+p_p\sin\beta\sigma_x), \tag{10}$$

with components parallel and perpendicular to the direction of the target polarization vector given by $p_p\cos\beta=\mathrm{tr}(\rho_{\rm in}\,\sigma_z)$ and $p_p\sin\beta=\mathrm{tr}(\rho_{\rm in}\,\sigma_x)$.

The spin density matrices for any target-positron system can now be obtained by taking direct products of the individual target and positron spin density matrices. For the singlet-positron system, with $\beta=0$,

$$\rho_{\rm in}=\tfrac{1}{2}(\varepsilon_2+p_p\sigma_z), \tag{11}$$

for the doublet-positron system, using Eqs. (8) and (10), we get

$$\begin{aligned}\rho_{\rm in}=\tfrac{1}{4}[&(\varepsilon_1\times\varepsilon_2)+p_p\cos\beta(\varepsilon_1\times\sigma_z)+p_p\sin\beta(\varepsilon_1\times\sigma_x)\\&+P_z(\sigma_z\times\varepsilon_2)+P_zp_p\cos\beta(\sigma_z\times\sigma_z)\\&+P_zp_p\sin\beta(\sigma_z\times\sigma_x)],\end{aligned} \tag{12}$$

and for the triplet-positron system, using Eqs. (9) and (10), we get

$$\begin{aligned}\rho_{\rm in}=\tfrac{1}{6}\big[&(E_1\times\varepsilon_2)+p_p\cos\beta(E_1\times\sigma_z)+p_p\sin\beta(E_1\times\sigma_x)\\&+\tfrac{3}{2}P_z(S_z\times\varepsilon_2)+\tfrac{3}{2}P_zp_p\cos\beta(S_z\times\sigma_z)\\&+\tfrac{3}{2}P_zp_p\sin\beta(S_z\times\sigma_x)+\tfrac{1}{2}P_{zz}(S_{zz}\times\varepsilon_2)\\&+\tfrac{1}{2}P_{zz}p_p\cos\beta(S_{zz}\times\sigma_z)+\tfrac{1}{2}P_{zz}p_p\sin\beta(S_{zz}\times\sigma_x)\big].\end{aligned} \tag{13}$$

The matrix elements of the outgoing density matrix given by Eq. (1) are obtained as follows:

$$\begin{aligned}&\langle S_iM_i|\langle S_dM_d|\rho_{\rm out}|S_iM_i''\rangle|S_dM_d''\rangle\\&\quad=\langle S_iM_i|\langle S_dM_d|\hat{M}|S_eM_e\rangle|S_pM_p\rangle\\&\qquad\times\langle S_eM_e|\langle S_pM_p|\rho_{\rm in}|S_eM_e''\rangle|S_pM_p''\rangle\\&\qquad\times\langle S_eM_e''|\langle S_pM_p''|\hat{M}^\dagger|S_iM_i''\rangle|S_dM_d''\rangle.\end{aligned} \tag{14}$$

We define projection operators P ($^{\rm para,ion}$) and P ($^{\rm ortho,ion}$), which pick out the para-positronium and ortho-positronium states formed *coincident* with a particular ion state. Specifically, $\langle S_iM_i|\ \langle S_dM_d|\ \rho_{\rm out}P\ (^{\rm para,ion})|S_i\ M_i''\rangle|S_d\ M_d''\rangle$ is nonzero only when $S_d=M_d=0$ for a specific S_i and M_i, while $\langle S_iM_i|\ \langle S_dM_d|\ \rho_{\rm out}P\ (^{\rm ortho,ion})|S_i\ M_i''\rangle|S_d\ M_d''\rangle$ is nonzero only when $S_d=1$ for a specific S_i and M_i. Using the projection operators and Eq. (14), we get

$$\begin{aligned}&\langle S_iM_i|\langle 00|\rho_{\rm out}P(^{\rm para,ion})|S_iM_i\rangle|00\rangle\\&\quad=\sum_{M_eM_p}\sum_{M_e''M_p''}\langle S_iM_i|\langle 00|\hat{M}|S_eM_e\rangle|S_pM_p\rangle\\&\qquad\times\langle S_eM_e|\langle S_pM_p|\rho_{\rm in}|S_eM_e''\rangle|S_pM_p''\rangle\\&\qquad\times\langle S_eM_e''|\langle S_pM_p''|\hat{M}^\dagger|S_iM_i\rangle|00\rangle\end{aligned} \tag{15}$$

and

$$\begin{aligned}&\langle S_iM_i|\langle 1M_d|\rho_{\rm out}P(^{\rm ortho,ion})|S_iM_i\rangle|1M_d\rangle\\&\quad=\sum_{M_d}\sum_{M_eM_p}\sum_{M_e''M_p''}\langle S_iM_i|\langle 1M_d|\hat{M}|S_eM_e\rangle|S_pM_p\rangle\\&\qquad\times\langle S_eM_e|\langle S_pM_p|\rho_{\rm in}|S_eM_e''\rangle|S_pM_p''\rangle\\&\qquad\times\langle S_eM_e''|\langle S_pM_p''|\hat{M}^\dagger|S_iM_i\rangle|1M_d\rangle.\end{aligned} \tag{16}$$

We compute the outgoing density matrices for the singlet, doublet, and triplet targets using Eq. (15) and Eq. (16) with the incoming density matrices given in Eqs. (11), (12), and (13), respectively. From the elements of the outgoing spin density matrices, we calculate the probabilities of forming para-positronium or ortho-positronium for a specific spin state of the outgoing target ion. We also calculate the probabilities for cases where the ion spins are not detected, by summing over S_i and M_i in Eqs. (15) and (16).

TABLE II. The para-positronium yields just after the collision at $t=0$, labeled $N_{\text{para}}(0)$, and the ortho-positronium yields just after the collision at $t=0$, labeled $N_{\text{ortho}}(0)$, for reactions in which a positron beam collides with a singlet, an unpolarized doublet, a polarized doublet with $M_e=\pm\frac{1}{2}$, an unpolarized triplet, or a polarized triplet with $M_e=\pm1$ or 0, to form para-positronium with $S_d=0$ or ortho-positronium with $S_d=1$. The outgoing singlet ion is in the $S_i=\frac{1}{2}$ state, the outgoing doublet ion can be in the $S_i=0$ or $S_i=1$ state, and the outgoing triplet ion can be in the $S_i=\frac{1}{2}$ or in the $S_i=\frac{3}{2}$ state. A factor of $|f^{S_e}|^2$ multiplies each term, with $S_e=0$, $\frac{1}{2}$, and 1 for the singlet, doublet, and triplet, respectively.

	$N_{\text{para}}(0)$	$N_{\text{ortho}}(0)$
Singlet		
$M_i=\pm\frac{1}{2}$	$\frac{1}{8}(1\pm p_p)$	$\frac{1}{8}(3\mp p_p)$
S_i, M_i undetected	$\frac{1}{4}$	$\frac{3}{4}$
Unpolarized Doublet		
$S_i=0\ M_i=0$	$\frac{1}{4}$	$\frac{3}{4}$
$S_i=1\ M_i=\pm1$	$\frac{1}{12}(1\pm p_p\cos\beta)$	$\frac{1}{12}(3\mp p_p\cos\beta)$
$S_i=1\ M_i=0$	$\frac{1}{12}$	$\frac{1}{4}$
Polarized Doublet		
$M_e=\pm\frac{1}{2}\ S_i=0\ M_i=0$	$\frac{1}{4}(1\mp \mathrm{p}_p\cos\beta)$	$\frac{1}{4}(3\pm p_p\cos\beta)$
$M_e=\pm\frac{1}{2}\ S_i=0\ M_i$ undetected	$\frac{1}{4}(1\mp p_p\cos\beta)$	$\frac{1}{4}(3\pm p_p\cos\beta)$
$M_e=+\frac{1}{2}\ S_i=1\ M_i=+1$	$\frac{1}{6}(1+p_p\cos\beta)$	$\frac{1}{6}(3-p_p\cos\beta)$
$M_e=+\frac{1}{2}\ S_i=1\ M_i=0$	$\frac{1}{12}(1-p_p\cos\beta)$	$\frac{1}{12}(3+p_p\cos\beta)$
$M_e=+\frac{1}{2}\ S_i=1\ M_i=-1$	0	0
$M_e=-\frac{1}{2}\ S_i=1\ M_i=+1$	0	0
$M_e=-\frac{1}{2}\ S_i=1\ M_i=0$	$\frac{1}{12}(1+p_p\cos\beta)$	$\frac{1}{12}(3-p_p\cos\beta)$
$M_e=-\frac{1}{2}\ S_i=1\ M_i=-1$	$\frac{1}{6}(1-p_p\cos\beta)$	$\frac{1}{6}(3+p_p\cos\beta)$
$M_e=\pm\frac{1}{2}\ S_i=1\ M_i$ undetected	$\frac{1}{12}(3\pm p_p\cos\beta)$	$\frac{1}{12}(9\mp p_p\cos\beta)$
$M_e=\pm\frac{1}{2}\ S_i, M_i$ undetected	$\frac{1}{6}(3\mp p_p\cos\beta)$	$\frac{1}{6}(9\pm p_p\cos\beta)$
Unpolarized Triplet		
$S_i=\frac{1}{2}\ M_i=\pm\frac{1}{2}$	$\frac{1}{24}(3\mp p_p\cos\beta)$	$\frac{1}{24}(9\pm p_p\cos\beta)$
$S_i=\frac{3}{2}\ M_i=\pm\frac{3}{2}$	$\frac{1}{16}(1\pm p_p\cos\beta)$	$\frac{1}{16}(3\mp p_p\cos\beta)$
$S_i=\frac{3}{2}\ M_i=\pm\frac{1}{2}$	$\frac{1}{48}(3\pm p_p\cos\beta)$	$\frac{1}{48}(9\mp p_p\cos\beta)$
Polarized Triplet		
$M_e=+1\ S_i=\frac{1}{2}\ M_i=+\frac{1}{2}$	$\frac{1}{4}(1-p_p\cos\beta)$	$\frac{1}{4}(3+p_p\cos\beta)$
$M_e=+1\ S_i=\frac{1}{2}\ M_i=-\frac{1}{2}$	0	0
$M_e=+1\ S_i=\frac{1}{2}\ M_i$ undetected	$\frac{1}{4}(1-p_p\cos\beta)$	$\frac{1}{4}(3+p_p\cos\beta)$
$M_e=+1\ S_i=\frac{3}{2}\ M_i=+\frac{3}{2}$	$\frac{3}{16}(1+p_p\cos\beta)$	$\frac{3}{16}(3-p_p\cos\beta)$
$M_e=+1\ S_i=\frac{3}{2}\ M_i=+\frac{1}{2}$	$\frac{1}{16}(1-p_p\cos\beta)$	$\frac{1}{16}(3+p_p\cos\beta)$
$M_e=+1\ S_i=\frac{3}{2}\ M_i=-\frac{1}{2}$	0	0
$M_e=+1\ S_i=\frac{3}{2}\ M_i=-\frac{3}{2}$	0	0
$M_e=+1\ S_i=\frac{3}{2}\ M_i$ undetected	$\frac{1}{8}(2+p_p\cos\beta)$	$\frac{1}{8}(6-p_p\cos\beta)$
$M_e=0\ S_i=\frac{1}{2}\ M_i=\pm\frac{1}{2}$	$\frac{1}{8}(1\pm p_p\cos\beta)$	$\frac{1}{8}(3\mp p_p\cos\beta)$
$M_e=0\ S_i=\frac{1}{2}\ M_i$ undetected	$\frac{1}{4}$	$\frac{3}{4}$
$M_e=0\ S_i=\frac{3}{2}\ M_i=\pm\frac{3}{2}$	0	0
$M_e=0\ S_i=\frac{3}{2}\ M_i=\pm\frac{1}{2}$	$\frac{1}{8}(1\pm p_p\cos\beta)$	$\frac{1}{8}(3\mp p_p\cos\beta)$
$M_e=0\ S_i=\frac{3}{2}\ M_i$ undetected	$\frac{1}{4}$	$\frac{3}{4}$
$M_e=-1\ S_i=\frac{1}{2}\ M_i=+\frac{1}{2}$	0	0
$M_e=-1\ S_i=\frac{1}{2}\ M_i=-\frac{1}{2}$	$\frac{1}{4}(1+p_p\cos\beta)$	$\frac{1}{4}(3-p_p\cos\beta)$
$M_e=-1\ S_i=\frac{1}{2}\ M_i$ undetected	$\frac{1}{4}(1+p_p\cos\beta)$	$\frac{1}{4}(3-p_p\cos\beta)$
$M_e=-1\ S_i=\frac{3}{2}\ M_i=+\frac{3}{2}$	0	0
$M_e=-1\ S_i=\frac{3}{2}\ M_i=+\frac{1}{2}$	0	0
$M_e=-1\ S_i=\frac{3}{2}\ M_i=-\frac{1}{2}$	$\frac{1}{16}(1+p_p\cos\beta)$	$\frac{1}{16}(3-p_p\cos\beta)$
$M_e=-1\ S_i=\frac{3}{2}\ M_i=-\frac{3}{2}$	$\frac{3}{16}(1-p_p\cos\beta)$	$\frac{3}{16}\ (3+p_p\cos\beta)$
$M_e=-1\ S_i=\frac{3}{2}\ M_i$ undetected	$\frac{1}{8}(2-p_p\cos\beta)$	$\frac{1}{8}(6+p_p\cos\beta)$
$M_e=+1\ S_i, M_i$ undetected	$\frac{1}{8}(4-p_p\cos\beta)$	$\frac{1}{8}(12+p_p\cos\beta)$
$M_e=0\ S_i, M_i$ undetected	$\frac{1}{2}$	$\frac{3}{2}$
$M_e=-1\ S_i, M_i$ undetected	$\frac{1}{8}(4+p_p\cos\beta)$	$\frac{1}{8}(12-p_p\cos\beta)$

III. RESULTS

We define the time just after the collision as $t=0$, and we consider the probabilities of forming para-positronium just after the collision, labeled $N_{\text{para}}(0)/N_{\text{total}}(0)$, and the probabilities of forming ortho-positronium just after the collision, labeled $N_{\text{ortho}}(0)/N_{\text{total}}(0)$. We calculate N_{para} (0) and N_{ortho} (0) from the outgoing spin density matrices, and we present them in Table II for all three types of targets. The values for N_{para} (0) and N_{ortho} (0) include a scattering amplitude factor $|f^{S_e}|^2$, with $S_e=0$, $\frac{1}{2}$, and 1 for the singlet, doublet, and triplet, respectively. With the number of outgoing ion states n equal to 1 for the singlet ($S_i=\frac{1}{2}$) and 2 for both the doublet ($S_i=0$ or 1) and the triplet ($S_i=\frac{1}{2}$ or $\frac{3}{2}$), we define

$$N_{\text{total}}(0)=n|f^{S_e}|^2. \tag{17}$$

First we use the probabilities to calculate the total positronium annihilation rate at $t=0$, defined as $\lambda_{\text{para}}\ [N_{\text{para}}(0)/N_{\text{total}}(0)]+\lambda_{\text{ortho}}[N_{\text{ortho}}(0)/N_{\text{total}}(0)]$, with the para-positronium annihilation rate λ_{para} equal to 8 ns^{-1} and the ortho-positronium annihilation rate λ_{ortho} equal to $\frac{1}{142}$ ns^{-1}. For example, from Table II, for the singlet with ion spin $M_i=\pm\frac{1}{2}$,

$$N_{\text{para}}(0)/N_{\text{total}}(0)=\tfrac{1}{8}(1\pm p_p) \tag{18}$$

and

$$N_{\text{ortho}}(0)/N_{\text{total}}(0)=\tfrac{1}{8}(3\mp p_p). \tag{19}$$

Without detection of the ion spins, the total probability, which is the sum of $N_{\text{para}}(0)/N_{\text{total}}(0)$ and $N_{\text{ortho}}(0)/N_{\text{total}}(0)$, equals 1 as expected.

Second, we present the ratios of para- to ortho-positronium yields at $t=0$, given as $N_{\text{para}}(0)/N_{\text{ortho}}(0)$. For example, from Table II, for the doublet with target spin $M_e=\pm\frac{1}{2}$ and ion spins $S_i=0$, $M_i=0$,

$$N_{\text{para}}(0)/N_{\text{ortho}}(0)=(1\mp p_p\cos\beta)/(3\pm p_p\cos\beta). \tag{20}$$

In Fig. 1 (see also Table III), we present the ratios $N_{\text{para}}(0)/N_{\text{ortho}}(0)$ for all three targets, using the values from Table II with $p_p=0.5$. Curves 1A and 1B represent the case of the doublet in Eq. (20). We consider the variation in the ratios of the para- to ortho-positronium yields as β ranges from 0° to 180°. The ratios vary from 0 to 1 for all the curves except curve 2, which is constant at $\frac{1}{3}$. In some cases, the ratios for forming one type of spin state are greater than those for the other. For example, for a polarized doublet target with spin $M_e=\frac{1}{2}$, $0<\beta<90°$, and no detection of the M_i spin, the ratio for forming the $S_i=1$ state (curve 3A) is greater than that for forming the $S_i=0$ state (curve 1B).

Finally, we consider the para-positronium and ortho-positronium yields as functions of time for the special case when $\beta=90°$. The yields N_{para} (t) and N_{ortho} (t), at time $t>0$, obtained from the decay law for each type of positronium, are given by

$$N_{\text{para}}(t)=N_{\text{para}}(0)e^{-\lambda_{\text{para}}t} \tag{21}$$

TABLE III. Properties of curves labeled 1A to 5B appearing in Fig. 1. The values are obtained from Table II with $p_p=0.5$. See Table II for curve details.

1A	unpolarized doublet, $S_i=1$, $M_i=1$
	polarized doublet, target spin $M_e=\frac{1}{2}$, $S_i=1$, $M_i=1$
	polarized doublet, target spin $M_e=-\frac{1}{2}$, $S_i=0$, M_i undetected or 0, or $S_i=1$, $M_i=0$
	unpolarized triplet, $S_i=\frac{3}{2}$, $M_i=\frac{3}{2}$
	polarized triplet, target spin $M_e=1$, $S_i=\frac{3}{2}$, $M_i=\frac{3}{2}$
	polarized triplet, target spin $M_e=0$, $S_i=\frac{1}{2}$, $M_i=\frac{1}{2}$, or $S_i=\frac{3}{2}$, $M_i=\frac{1}{2}$
	polarized triplet, target spin $M_e=-1$, $S_i=\frac{1}{2}$, M_i undetected or $-\frac{1}{2}$, or $S_i=\frac{3}{2}$, $M_i=-\frac{1}{2}$
1B	unpolarized doublet, $S_i=1$, $M_i=-1$
	polarized doublet, target spin $M_e=\frac{1}{2}$, $S_i=0$, M_i undetected or 0, or $S_i=1$, $M_i=0$
	polarized doublet, target spin $M_e=-\frac{1}{2}$, $S_i=1$, $M_i=-1$
	unpolarized triplet, $S_i=\frac{3}{2}$, $M_i=-\frac{3}{2}$
	polarized triplet, target spin $M_e=1$, $S_i=\frac{1}{2}$, M_i undetected or $\frac{1}{2}$, or $S_i=\frac{3}{2}$, $M_i=\frac{1}{2}$
	polarized triplet, target spin $M_e=0$, $S_i=\frac{1}{2}$, $M_i=-\frac{1}{2}$, or $S_i=\frac{3}{2}$, $M_i=-\frac{1}{2}$
	polarized triplet, target spin $M_e=-1$, $S_i=\frac{3}{2}$, $M_i=-\frac{3}{2}$
2	unpolarized doublet, $S_i=0$, $M_i=0$, $S_i=1$, $M_i=0$
	polarized triplet, target spin $M_e=0$, $S_i=\frac{1}{2}$, M_i undetected, or $S_i=\frac{3}{2}$, M_i undetected
	polarized triplet, target spin $M_e=0$, S_i, M_i undetected
3A	polarized doublet, target spin $M_e=\frac{1}{2}$, $S_i=1$, M_i undetected
	polarized doublet, target spin $M_e=-\frac{1}{2}$, S_i, M_i undetected
	unpolarized triplet, $S_i=\frac{1}{2}$, $M_i=-\frac{1}{2}$, or $S_i=\frac{3}{2}$, $M_i=\frac{1}{2}$
3B	polarized doublet, target spin $M_e=-\frac{1}{2}$, $S_i=1$, M_i undetected
	polarized doublet, target spin $M_e=\frac{1}{2}$, S_i, M_i undetected
	unpolarized triplet, $S_i=\frac{1}{2}$, $M_i=\frac{1}{2}$, or $S_i=\frac{3}{2}$, $M_i=-\frac{1}{2}$
4A	polarized triplet, target spin $M_e=1$, $S_i=\frac{3}{2}$, M_i undetected
4B	polarized triplet, target spin $M_e=-1$, $S_i=\frac{3}{2}$, M_i undetected
5A	polarized triplet, target spin $M_e=-1$, S_i, M_i undetected
5B	polarized triplet, target spin $M_e=1$, S_i, M_i undetected

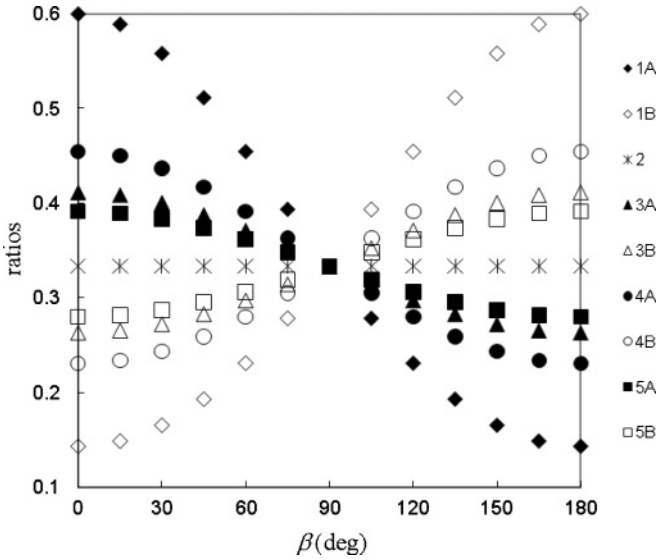

FIG. 1. The ratios $N_{\text{para}}(0)/N_{\text{ortho}}(0)$ for the unpolarized and polarized doublet and the unpolarized and polarized triplet. The values are obtained from Table II with $p_p = 0.5$. The curves labeled 1A–5B represent the cases given in Table III.

and

$$N_{\text{ortho}}(t) = N_{\text{ortho}}(0)e^{-\lambda_{\text{ortho}}t}. \tag{22}$$

We represent the values of N_{para} (0) and N_{ortho} (0) from Table II for the doublet and triplet targets as $\frac{(\text{integer})}{48}|f^{S_e}|^2$ and $\frac{(\text{integer})}{16}|f^{S_e}|^2$, respectively. For the doublet, integer = 4, 8, 12, or 24, and for the triplet, integer = 3, 6, 9, 12, or 24. Equations (21) and (22) can now be recast so that $\ln[N_{\text{para}}(0)]$ and $\ln[N_{\text{ortho}}(0)]$ become intercepts in straight-line equations of the form

$$\ln N_{\text{para}}(t) = \ln\left(\frac{(\text{integer})}{48}|f^{S_e}|^2\right) - \lambda_{\text{para}}t \tag{23}$$

and

$$\ln N_{\text{ortho}}(t) = \ln\left(\frac{(\text{integer})}{16}|f^{S_e}|^2\right) - \lambda_{\text{ortho}}t. \tag{24}$$

As noted earlier, para- and ortho-positronium differ in their spin (0 for para and 1 for ortho), types of decay (two-photon for para and three-photon for ortho), and annihilation rates ($8\,\text{ns}^{-1}$ for para and $\frac{1}{142}$ ns^{-1} for ortho). These differences are manifested in Eqs. (18)–(20), (23), and (24) and provide a specific experimental tool for the detection of the spins of the final states.

IV. CONCLUSION

We have described a method to calculate ratios of para- to ortho-positronium yields as well as probabilities for the formation of para- and ortho-positronium in coincidence with a target ion, in the collision of a polarized positron beam with three types of targets. We have considered unpolarized and polarized targets and all possible ion spin states. We have given the ratios and probabilities as functions of the angle β. We have presented the ratios of para-positronium to ortho-positronium yields as well as total positronium annihilation rates, at $t = 0$, as functions of β. We have also presented the para-positronium and ortho-positronium yields as functions of time, for fixed β.

Some of the spin structures considered in the electron scattering and nuclear physics processes in Refs. [10–15] are similar to those in our work. The techniques that we adopted from Ref. [3] have also been used in Refs. [10–15] for polarized electron-atom scattering and in nuclear processes involving polarized proton, neutron, deuteron, and triton beams and polarized proton and deuteron targets. However, an important difference between polarized positron-atom collisions and polarized electron-atom collisions is that positronium formation can occur only with positron collisions, while elastic scattering, excitation, and ionization can occur with both positron and electron collisions [17]. The nuclear physics interactions are strongly spin dependent, and therefore we expect the scattering-matrix elements in those cases to depend on more than just Racah coefficients, unlike our work, in which the entire spin dependence is in the recoupling coefficients. Furthermore, since para-positronium and ortho-positronium have different spins, types of decay, and rates of decay, positron-atom collisions in which both types of positronium are formed are useful for experimental detection of the spins of the final states. For these reasons, the positron-atom collision process with the production of positronium and an atomic ion, studied here, is unique and differs from both polarized electron-atom scattering as well as nuclear interactions.

Spin effects were a focus of a 1985 Positron Workshop [18], and since then there have been considerable advances in the development of intense polarized positron beams [19–21]. Reference [22] gives a comprehensive compilation of theoretical and experimental research in the field of positron physics. Measurements of differential cross sections for positronium formation made during positronium beam-development experiments, as well as positron-argon and positron-krypton collisions in which positronium is detected in coincidence with the atomic ion, are presented [22]. Theoretical calculations which are most relevant to our study include positron-hydrogen and positron-helium scattering. Cross sections for total positronium formation as well as for the formation of the positronium states, $1s$, $2s$, and $2p$, for positron-hydrogen scattering in the energy range 0–110 eV, calculated using a 33-state approximation, are presented in Ref. [23]. Total positronium formation cross sections for positron-helium scattering in the Ore gap (17.78–20.58 eV), calculated using the Kohn variational method, are given in Ref. [24]. Cross sections for total positronium formation as well as for the formation of the positronium states, $1s$, $2s$, and $2p$, for positron-helium scattering in the energy range above the positronium formation threshold of 17.78 eV, calculated using coupled-pseudostate methods, are presented in Ref. [25].

In this article, we have not calculated differential cross sections or polarization vectors for the outgoing ions, which could be useful for specifying their direction. Differential cross sections can be calculated using the density matrices given by Eqs. (11)–(14) and Eq. (14.72) in Ref. [26] or Eq. (12) in Chap. 55 of Ref. [1], while polarization vectors can be calculated using Eqs. (11)–(14) and Eq. (13) in Chap. 55 of Ref. [1]. Our focus in this work is to provide some motivation for experiments to look for para- and

ortho-positronium yields separately, as well as for positronium formation in coincidence with specific spin states of the outgoing ion. We would like to postpone calculations of observables such as differential cross sections and polarization vectors, with comparisons to relevant quantities in theoretical and experimental studies of positron-hydrogen scattering or positron-helium scattering, to the future. Our next step is to study positronium quenching and dissociative attachment. The positronium-quenching process can be described as target + positronium → target + positronium. If an ortho-positronium beam is used, both para- and ortho-positronium can be formed in the final state. In the dissociative-attachment process described as target molecule + positron → target atom + positronium oxide, both para- and ortho-positronium oxides can be formed in the final state. The technique described in this article can be very easily used to calculate positronium yields for the quenching process or positronium-oxide yields for the dissociative-attachment process.

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