Symmetry of Dipositronium Ps_2

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We work out the complete symmetry and spin problem for diatomic positronium Ps_2 for the ground and singly excited states of zero orbital angular momentum. The general form of the wave function for each state is given, with due regard to charge conjugation parity. Annihilation rates are discussed, and correlations to dissociation products are deduced. We indicate how the approach is extensible to larger aggregates: i.e., $PsPs_n$, $n > 2$.

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The basic physics of diatomic positronium was elucidated by Wheeler in 1946 [1]. It was soon shown to be stable to dissociation from two positronium atoms by a variational calculation [2]. Since then about 50 authors have improved upon this first result, and today the binding energy stands at 0.435 485 eV [3]. Spin was not explicitly considered in most of these calculations, and in most cases the symmetry of the spatial part of the wave function was deduced, not always correctly, from plausibility arguments. The first attempt to give a comprehensive treatment of spatial symmetry was made only ten years ago [4].

The Bose-Einstein condensation (BEC) of positronium is thought to proceed through Ps_2 [5]. There is considerable current interest in positronium BEC [6] as well as in resonance states of Ps_2 [7] and in Ps-Ps scattering [8]. The confirmation of the formation of Ps_2 depends upon the measurement of some well-understood property [3]. Not all the states of Ps_2 are bound in field-free regions, but this may not be true in the presence of external fields [9,10]. For these reasons we need accurate wave functions, including the spin dependence, for all possible states.

In the present work the spin part of the wave function is treated exactly and the correct symmetry of the total wave function is deduced from first principles. We work in the nonrelativistic Schrödinger picture and use the spin-free Hamiltonian:

$$\hat{H} = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2 + \nabla_3^2 + \nabla_4^2) - \left(\frac{1}{r_{13}} + \frac{1}{r_{14}} + \frac{1}{r_{23}} + \frac{1}{r_{24}}\right) + \left(\frac{1}{r_{12}} + \frac{1}{r_{34}}\right). \quad (1)$$

Electrons are arbitrarily labeled 1 and 2, and positrons, 3 and 4. We use atomic units. In the present work we consider ground and first excited states of zero orbital angular momentum. The total spin operators $\hat{S}^2$ and $\hat{S}_z$ give good quantum numbers S and M.

Consider four points arbitrarily placed in four-dimensional (Cartesian plus spin) space. We label them a, b, c, and d. To establish a reference system, we initially put particle 1 at point a, particle 2 at b, and so forth. The points in spin space, $m = \pm\frac{1}{2}$, are denoted by the familiar spin functions α and β, whose arguments denote particles. But spatial functions do not denote particles but, rather, points in space that can be occupied by any in a set of interchangeable particles. We accommodate this difference by using two kinds of particle interchange operators: those that interchange two designated particles regardless of where they are in space (denoted as, e.g., $\hat{P}_{12}$) and those that interchange whichever two particles sit on designated points in space (e.g., $\hat{Q}_{ab}$). This distinction has been clarified by Bunker and Howard [11]. Interchange operators of the first kind follow the convention of Bunker [12,13] and those of the second kind, of Wigner [14]. The Hamiltonian commutes with these interchangers of like particles, as well as with interchangers of unlike particles (e.g., $\hat{P}_{13}\hat{P}_{24}$ and $\hat{Q}_{ac}\hat{Q}_{bd}$). One can think of other commuting particle interchange operators, but there are only three independent group generators among them. Kinghorn and Poshusta (KP) chose a particular set in their study of spatial symmetry of the wave functions. Here we illustrate another choice, one that accounts for spin and appears to be arbitrarily extensible to larger aggregates of positronium atoms.

$\hat{P}_{13}\hat{P}_{24}$ and $\hat{Q}_{ac}\hat{Q}_{bd}$ remind us of charge conjugation from quantum electrodynamics (QED). They also remind us of the inversion operator E^* that was used by Longuet-Higgins in his study of the symmetry properties of nonrigid molecules [15]. Ps_2 is the ultimate nonrigid molecule, and we apply the theory of permutation groups as used for nonrigid molecules [13] to the present problem. We define a four-space particle interchange operator that accommodates the notational differences between space and spin by exploiting the distinction between the Bunker and Wigner conventions:

$$\hat{R}_{12} = (\hat{P}_{12})_{3\text{-space}}(\hat{Q}_{ab})_{\text{spin}}. \quad (2)$$

We denote the group $\{\hat{E}, \hat{R}_{12}\}$ as $S_2^{(e^-)}$. It is the electron interchange group in four-space. We similarly define $S_2^{(e^+)}$ for the positrons. We define a subgroup $\mathcal{T}_2^{(2-ep)}$ to accommodate electron-positron interchange:

$$\hat{R}_{ep} = (\hat{Q}_{ep})_{3\text{-space}}(\hat{P}_{ep})_{\text{spin}}, \quad (3)$$

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$$\mathcal{T}_2^{(2-ep)} = \{\hat{E}, \hat{R}_{ep}\}. \tag{4}$$

The direct product

$$\mathcal{G}(\mathrm{Ps}_2) = \mathcal{S}_2^{(e^-)} \otimes \mathcal{S}_2^{(e^+)} \otimes \mathcal{T}_2^{(2-ep)} \tag{5}$$

is the permutation group for Ps_2. This group is isomorphous with the molecular point group D_{2h} and with the permutation group G_8 [13]. The character table can be constructed from the associations given in Table I. It is important to recognize that the theory of nonrigid molecules requires the permutation group of Ps_2 to be factorable as in Eq. (5) [13,15]. The group to which KP were led by their choice of group generators is not factorable.

One can create a function of the coordinates of particles of Ps_2 that has any desired symmetry by applying the projection operator

$$\hat{\mathcal{R}}_{p,q,c} = (1 + c\hat{R}_{ep})(1 + q\hat{R}_{34})(1 + p\hat{R}_{12}) \tag{6}$$

to a function of space and spin variables. If the function is to serve as a trial wave function for Ps_2 then it must, of course, have $p = q = -1$. The value of c is less well understood, at least by this author. We are tempted to identify it as C, the charge conjugation quantum number from QED, but we know of no experimental justification for this. We leave the question open.

To form a wave function, we project the proper symmetry from a primitive function with a projection operator of the form (6)

$$\hat{\mathcal{R}}_{-1,-1,c}\{F(r_{13}, r_{14}, r_{23}, r_{24}, r_{12}, r_{34})\Gamma^{(C)}_{SM,S_eS_p}(1, 2, 3, 4)\}. \tag{7}$$

The primitive function is the product of spatial and spin factors that have no particular particle interchange symmetry, but the spin function is an eigenfunction of the total spin operators $\hat{S}^2$ and $\hat{S}_z$. S_e and S_p are the total spin quantum numbers for the electrons and positrons separately. The arguments of F are interparticle distances.

Each state of Ps_2 possesses definite charge conjugation and inversion parities. The inversion parities of the states considered here are even. The charge conjugation C follows by writing spin functions as products of those of two positronium atoms [5]. For convenience we choose a different but equally valid way: We combine spin eigenfunctions of two electrons with those of two positrons in all possible ways. In Table II we give the spin functions for defined S_e and S_p used here as well as the spin functions of Ref. [5]. In Table III we give the spin functions that appear in Eq. (7) in terms of both schemes. Only states with $M = S$ are given; the rest are obvious. From Table III we can read off the values of C for our spin functions, and we see that S_e and S_p are, indeed, not good quantum numbers. However, we still need these two quantities as a notational device in order to distinguish between states that have the same set of values for S, M, and C.

TABLE I. Operators and characters for $\mathcal{G}(\mathrm{Ps}_2)$, and the effect of the operators on space (third row) and spin arguments (fourth row) in wave functions. The order of points is always *abcd*.

$\hat{E}$	$\hat{R}_{12}$	$\hat{R}_{34}$	$\hat{R}_{34}\hat{R}_{12}$	$\hat{R}_{ep}$	$\hat{R}_{ep}\hat{R}_{12}$	$\hat{R}_{ep}\hat{R}_{34}$	$\hat{R}_{ep}\hat{R}_{34}\hat{R}_{12}$
1	p	q	pq	c	pc	qc	pqc
1234	2134	1243	2143	3412	3421	4312	4321
1234	2134	1243	2143	3412	4312	3421	4321

For a concise discussion, we define a column vector of spatial functions produced by operating on F in Eq. (7) with each of the operators in Table I in turn:

$$\mathsf{F} = \begin{bmatrix} F(r_{13}, r_{14}, r_{23}, r_{24}, r_{12}, r_{34}) \\ F(r_{23}, r_{24}, r_{13}, r_{14}, r_{12}, r_{34}) \\ F(r_{14}, r_{13}, r_{24}, r_{23}, r_{12}, r_{34}) \\ F(r_{24}, r_{23}, r_{14}, r_{13}, r_{12}, r_{34}) \\ F(r_{13}, r_{23}, r_{14}, r_{24}, r_{34}, r_{12}) \\ F(r_{23}, r_{13}, r_{24}, r_{14}, r_{34}, r_{12}) \\ F(r_{14}, r_{24}, r_{13}, r_{23}, r_{34}, r_{12}) \\ F(r_{24}, r_{14}, r_{23}, r_{13}, r_{34}, r_{12}) \end{bmatrix}. \tag{8}$$

The result of operating with $\hat{\mathcal{R}}_{p,q,c}$ on F can now be written succinctly:

$$\hat{\mathcal{R}}_{p,q,c}F = [1\ p\ q\ pq\ c\ pc\ qc\ pqc]\mathsf{F} \equiv \mathcal{F}_{p,q,c}. \tag{9}$$

For states that have space-spin factorable wave functions, each factor has its own set of values of p, q, and c. To ensure the correct overall symmetry for such wave functions, we require that the product of the two p's and the two q's be -1. In any case, we denote wave functions as Ψ_{i,c_i}, where i, the same as the index in Table III, denotes all the quantum numbers except c_i.

We illustrate our method by an example. The interparticle coordinates that occupy a given argument position of

TABLE II. The spin functions (with defined S_e and S_p) used here, and those of Ref. [5] (with defined C and P).

$\|SMS_eS_p\rangle$	Present scheme
$\|0000\rangle$	$\|00\rangle_{12}\|00\rangle_{34}$
$\|1101\rangle$	$\|00\rangle_{12}\|11\rangle_{34}$
$\|1110\rangle$	$\|11\rangle_{12}\|00\rangle_{34}$
$\|2211\rangle$	$\|11\rangle_{12}\|11\rangle_{34}$
$\|1111\rangle$	$\frac{1}{\sqrt{2}}(\|11\rangle_{12}\|10\rangle_{34} - \|10\rangle_{12}\|11\rangle_{34})$
$\|0011\rangle$	$\frac{1}{\sqrt{3}}(\|11\rangle_{12}\|1,-1\rangle_{34} - \|10\rangle_{12}\|10\rangle_{34} + \|1,-1\rangle_{12}\|11\rangle_{34})$
$\|SMCP\rangle$	Platzman-Mills [5] scheme
$\|00++\rangle_s$	$\|00\rangle_{13}\|00\rangle_{24}$
$\|11-+\rangle$	$\frac{1}{\sqrt{2}}(\|11\rangle_{13}\|00\rangle_{24} + \|00\rangle_{13}\|11\rangle_{24})$
$\|11--\rangle$	$\frac{1}{\sqrt{2}}(\|11\rangle_{13}\|00\rangle_{24} - \|00\rangle_{13}\|11\rangle_{24})$
$\|22++\rangle$	$\|11\rangle_{13}\|11\rangle_{24}$
$\|11+-\rangle$	$\frac{1}{\sqrt{2}}(\|11\rangle_{13}\|10\rangle_{24} - \|10\rangle_{13}\|11\rangle_{24})$
$\|00++\rangle_t$	$\frac{1}{\sqrt{3}}(\|11\rangle_{13}\|1,-1\rangle_{24} - \|10\rangle_{13}\|10\rangle_{24} + \|1,-1\rangle_{13}\|11\rangle_{24})$

TABLE III. The spin functions of the present work in terms of the two schemes given in Table II. The index i connects space and spin factors of wave functions for the various states in the discussion below.

i	$\Gamma^{(C)}_{SM,S_eS_p}$	$\lvert SMS_eS_p\rangle$	$\lvert SMCP\rangle$
1	$\Gamma^{(+)}_{00,00}$	$\lvert 0000\rangle$	$\frac{\sqrt{3}}{2}\lvert 00++\rangle_t + \frac{1}{2}\lvert 00++\rangle_s$
2	$\Gamma^{(+)}_{11}$	$\frac{1}{\sqrt{2}}(\lvert 1110\rangle + \lvert 1101\rangle)$	$\lvert 11+-\rangle$
3	$\Gamma^{(-)}_{11}$	$\frac{1}{\sqrt{2}}(\lvert 1110\rangle - \lvert 1101\rangle)$	$\lvert 11--\rangle$
4	$\Gamma^{(+)}_{22,11}$	$\lvert 2211\rangle$	$\lvert 22++\rangle$
5	$\Gamma^{(-)}_{11,11}$	$\lvert 1111\rangle$	$\lvert 11-+\rangle$
6	$\Gamma^{(+)}_{00,11}$	$\lvert 0011\rangle$	$-\frac{1}{2}\lvert 00++\rangle_t + \frac{\sqrt{3}}{2}\lvert 00++\rangle_s$

each F in Eq. (8) are in general different, but the functional meaning is the same. We call each argument position a "functionality," and denote it by the positions in space that it represents, i.e., ab. We form a grid of the spatial coordinates for each functionality. These are the subscripts in Eq. (8). To each row of the grid we attach a spin function with coordinates as listed in Table I, and a multiplying coefficient for $p = q = -1$ and c undetermined. We can write the general form of the wave function for each state, which is the principal result of the present work. The wave function associated with the first spin factor in Table III is

$$\Psi_{1,c_1} = \mathcal{F}_{1,1,c_1}\Gamma^{(+)}_{00,00}. \tag{10}$$

The wave functions associated with the last three spin functions in Table III are

$$\Psi_{4,c_4} = \mathcal{F}_{-1,-1,c_4}\Gamma^{(+)}_{22,11}, \tag{11}$$

$$\Psi_{5,c_5} = \mathcal{F}_{-1,-1,-c_5}\Gamma^{(-)}_{11,11}, \tag{12}$$

$$\Psi_{6,c_6} = \mathcal{F}_{-1,-1,c_6}\Gamma^{(+)}_{00,11}. \tag{13}$$

When we apply $\hat{\mathcal{R}}_{-1,-1,c}$ to the product of F and the second and third spin functions in Table III, we arrive at functions that are mixtures of two different charge conjugations. We recover eigenfunctions of C if we constrain F in either of two ways: (1) we require the second and third arguments to be interchangeable (by making the functionalities ad and bc equivalent), or (2) the first and fourth arguments are interchangeable. In both cases, the fifth and sixth arguments are also made to be interchangeable. Then a disposable parameter appears in the wave function. One way of writing them is

$$\Psi_{2,1} = \mathcal{F}^{(1)}_{-1,1,1}\Gamma^{(+)}_{11}, \tag{14}$$

$$\Psi_{3,-1} = \mathcal{F}^{(1)}_{-1,1,1}\Gamma^{(-)}_{11}, \tag{15}$$

$$\Psi_{2,-1} = \mathcal{F}^{(2)}_{-1,1,-1}\Gamma^{(+)}_{11}, \tag{16}$$

$$\Psi_{3,1} = \mathcal{F}^{(2)}_{-1,1,-1}\Gamma^{(-)}_{11}, \tag{17}$$

where (1) and (2) denote the first or second set of constraints described above.

The wave functions given in Eqs. (10)–(17) are evidently of the most general form. We see that they are all space-spin factorable, and that S_e and S_p are not, in general, good quantum numbers. The energies of these states are determined by the subscripts of the spatial factors. The wave function given in Eq. (10) has no nodes at all if $c_1 = 1$. This must be the wave function for the ground state. We see that if $c_4 = -c_5 = c_6$ in Eqs. (11)–(13), the three states are degenerate except for a small hyperfine splitting. The two states whose wave functions are given by Eqs. (14) and (15) are similarly degenerate, as are those with the wave functions in Eqs. (16) and (17).

To a good approximation, the annihilation rate of a system is the expectation value of the operator [16]:

$$8\pi a_0^3 \sum_{e,p}\sum_{s,m} D_s \lvert s, m\rangle_{e,p}\,\delta^3(\boldsymbol{r}_{ep})\langle s, m\rvert_{e,p}. \tag{18}$$

The sums are over electron-positron pairs and their two-particle spin functions. $D_0 \sim 8\ \mathrm{ns}^{-1}$, $D_1 \sim 7\ \mu\mathrm{s}^{-1}$, and the others are negligible. Order-of-magnitude precision suffices for present purposes. For a system with a spin-space factorable wave function, the annihilation rate is the product of the electron-positron contact density, $\rho_{i,c_i} = \langle \Psi_{i,c_i} \lvert \delta^3(\boldsymbol{r}_{ep}) \rvert \Psi_{i,c_i}\rangle$, and a factor from the spin integrations that can be deduced from Tables II and III. The results are given in Table IV.

The density factors ρ_{i,c_i} depend strongly on the symmetry numbers of the spatial factors, so little can be said about λ without an accurate wave function.

We study the dissociation products of the states by examining the limiting forms of their general wave functions. By moving the points a, b, c, and d, we can make selected functionalities represent isolated positronium atoms. We can study the dissociation product $e^{\pm} + e^{\mp}\mathrm{Ps}$ in a similar way. The results are given in Table V. Tight binding forms can also be examined. The lowest possible energy of any state must be nodeless and have a wave function that has equivalent functionalities for all

TABLE IV. Annihilation rates λ for the states of Ps_2.

Ψ_{i,c_i}	$\lambda/(4 \times 8\pi a_0^3 \rho_{i,c_i})$		Note[a]
Ψ_{1,c_1}	$\frac{1}{4}D_0 + \frac{3}{4}D_1$	$\sim$	2
Ψ_{2,c_2}	D_1	$\sim$	0.007
Ψ_{3,c_3}	$\frac{1}{2}(D_0 + D_1)$	$\sim$	4
Ψ_{4,c_4}	D_1	$\sim$	0.007
Ψ_{5,c_5}	$\frac{1}{2}(D_0 + D_1)$	$\sim$	4
Ψ_{6,c_6}	$\frac{3}{4}D_0 + \frac{1}{4}D_1$	$\sim$	6

[a] This column is not λ, but rather denotes the result of a spin integration for one electron-positron pair, i.e., $\frac{1}{4}D_0 + \frac{3}{4}D_1 \sim 2\ \mathrm{ns}^{-1}$.

TABLE V. Dissociation limits for the wave functions of Ps_2 for different choices of the symmetry number c. "o" and "p" denote *ortho*- and *para*-positronium.

	Ps + Ps		$e^{\pm} + e^{\mp}$Ps	
	$c_i = C$	$c_i = -C$	$c_i = C$	$c_i = -C$
Ψ_{1,c_1}	$\frac{3}{4}o, o + \frac{1}{4}p, p$	$\frac{3}{4}o, o^{b} + \frac{1}{4}p, p^{b}$	Yes	Yes
Ψ_{2,c_2}	o, o^{a}	o, o^{a}	Yes	Yes
Ψ_{3,c_3}	o, p^{a}	o, p^{a}	Yes	Yes
Ψ_{4,c_4}	o, o	o, o^{b}	No	No
Ψ_{5,c_5}	o, p	o, p^{b}	No	No
Ψ_{6,c_6}	$\frac{1}{4}o, o + \frac{3}{4}p, p$	$\frac{1}{4}o, o^{b} + \frac{3}{4}p, p^{b}$	No	No

[a] One positronium atom is its $2s$ state.
[b] One positronium atom is its $2p$ state.

the attractive pairs, and for the negative pairs. Only the wave function $\Psi_{1,1}$ passes this test.

Because of space limitations, we confine our discussion of the literature on Ps_2 energy level calculations to a single paper, that of KP, which has guided subsequent workers. We label the irreducible representations of $\mathcal{G}(Ps_2)$ with the symmetry numbers of the spatial factor of the wave function, $[p, q, c]$. The A_1 state of KP appears to be $[1, 1, 1]$. Using the contact density of KP, we find its annihilation rate to be 4.4 ns^{-1}. KP report 1.1 ns^{-1}. Their B_1 state corresponds to the three degenerate $[-1, -1, 1]$ states, those with $i = 4$, 5, and 6. They are unbound in the absence of external fields, approaching two ground state Ps atoms. Our calculation of their annihilation rates, 0.014, 7.8, and 11.6 ns^{-1}, respectively, is consistent with the dissociation products shown in Table V. The B_2 state is $[1, 1, -1]$, and we find its annihilation rate to be 2.2 ns^{-1}. This state, with the wave function $\Psi_{1,-1}$, has $C = 1$. If it turns out that the symmetry number c_i is C, this state does not exist. The same conclusion applies to KP's A_2 state, which corresponds to three states, those with wave functions $\Psi_{4,-1}$, $\Psi_{5,1}$, and $\Psi_{6,-1}$. The E state of KP, which they find to be bound, appears to have a wave function that is a mixture of $\Psi_{2,1}$ and $\Psi_{3,-1}$. From Eqs. (14) and (15), we see that this combination does not have a well-defined charge conjugation quantum number and, hence, is not a state of the system.

The way is clear to extend Eq. (5) to larger aggregates of positronium. The permutation group

$$\mathcal{G}(Ps_n) = S_n^{(e^-)} \otimes S_n^{(e^+)} \otimes \mathcal{T}_2^{(n-ep)}, \qquad (19)$$

where $\mathcal{T}_2^{(n-ep)}$ is as defined in Eq. (4) with $\hat{R}_{ep}$ generalized to an n-fold product of pairwise electron-positron interchangers of the form of Eq. (3). $\mathcal{G}(Ps_n)$ is of the order $2(n!)^2$, and Ps_n has 2^{2n} spin states. $\mathcal{G}(Ps_3)$ has 2 four-dimensional, 8 two-dimensional, and 8 one-dimensional irreducible representations. Ps_3 has one spin state with $S = 3$ and $C = -1$, three have $S = 2$ with $C = 1$ and two with $C = -1$, three have $S = 1$ with $C = 1$ and six with $C = -1$, and four have $S = 0$ with $C = 1$ and one with $C = -1$.

A complete description of this work is now in preparation. Part of this work was presented at a meeting and will appear as a brief report [6], which this Letter supersedes. The author is grateful to M. E. Fajardo for asking just the right question, and to A. P. Mills, Jr., and R. J. Drachman for helpful comments. A portion of this work was done at the University of Florida Graduate Engineering and Research Center, Shalimar, Florida. This work is supported in part by the Air Force Research Laboratory, Eglin Air Force Base, Florida, USA.

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