1)

86(5): Quantum Mechanics of Positronium

The positronium "atom" is generally considered as H - ℓ and is described non-relativistically by:

$$H\phi = E\phi \qquad (1)$$

where

$$H = -\frac{\hbar^2\nabla^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} \qquad (2)$$

and

$$m = \frac{m_e m_p}{m_e + m_p}. \qquad (3)$$

Here

$$m_e = m_p \qquad (4)$$

so

$$m = \frac{1}{2} m_e. \qquad (5)$$

In this notation, m is the reduced mass, m_e and m_p are the electron and positron masses. The distance between the electron and positron is r. The complete wave function is:

$$\phi = \phi_e \phi_p. \qquad (6)$$

The Coulombic potential energy of positronium is therefore

$$V = -\frac{\alpha}{r} \text{ cm}^{-1} \text{ (wavenumbers)} \qquad (7)$$

and its ~~ex~~ total energy is quantized as follows

$$E = -\frac{rV}{2n^2 a} \text{ cm}^{-1} \text{ (wavenumbers)} \qquad (8)$$

Here α is the fine structure constant, a is the Bohr radius, and n is the principal quantum number.

2) <u>Spin-Spin Interaction</u>

In the case of positronium the electron and positron are two fermions with spins $s = 1/2$ (Atkins p. 121). Therefore the total angular momentum state is made up of

$$\alpha = |\tfrac{1}{2}, \tfrac{1}{2}\rangle, \quad \beta = |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \quad - (9)$$

In the <u>uncoupled representation</u> the electron and positron may be in any of the four states $|s_1 m_{s1}; s_2 m_{s2}\rangle$ with:

$$m_{s1} = \pm\frac{1}{2}, \quad m_{s2} = \pm\frac{1}{2} \quad - (10)$$

These four are:

$$|\tfrac{1}{2}, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}\rangle = \alpha_1 \alpha_2 \quad - (11)$$

$$|\tfrac{1}{2}, \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}\rangle = \alpha_1 \beta_2 \quad - (12)$$

$$|\tfrac{1}{2}, -\tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}\rangle = \beta_1 \alpha_2 \quad - (13)$$

$$|\tfrac{1}{2}, -\tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}\rangle = \beta_1 \beta_2. \quad - (14)$$

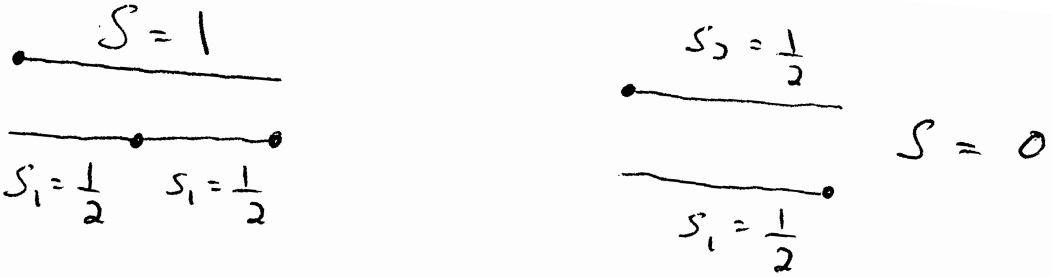
The individual angular momenta lie at unspecified positions, and the total angular momentum is indeterminate.

In <u>the coupled representation</u> the total spin angular momentum is S, the capital letter being used to denote angular momenta of collections of particles. In positronium it takes the value:

$$S = 0, 1 \quad - (15)$$

as follows.

3)



When $S = 0$ the only possible value of its Z component is $M_S = 0$. This is called a singlet and is called para-positronium. When $S = 1$, $M_S = 1, 0, -1$ and this is called a triplet state, ortho-positronium. Thus:

Para Positronium

$$|s_1 s_2; S M_s\rangle = |\tfrac{1}{2}, \tfrac{1}{2}; 0, 0\rangle \quad -(16)$$

Ortho Positronium

$$|s_1 s_2, S M_s\rangle = |\tfrac{1}{2}, \tfrac{1}{2}, 1, M_s\rangle \quad -(17)$$

The angular momentum state $|j_1 j_2; j m_j\rangle$ contains all values of m_{j1} and m_{j2} such that

$$m_{j1} + m_{j2} = m_j \quad -(18)$$

Therefore the coupled state is the sum over the uncoupled states $|j_1 m_{j1}; j_2 m_{j2}\rangle$ which conform to Eq. (18). The state $|\tfrac{1}{2}, \tfrac{1}{2}; 1, 0\rangle$ is sum of $\alpha_1 \beta_2$ and $\beta_1 \alpha_2$, because each corresponds to $M_s = 0$. In general

4)

$$|j_1 j_2 ; j m_j\rangle = \sum_{m_{j1}} \sum_{m_{j2}} C_{m_{j1}, m_{j2}} |j_1 m_{j1} ; j_2 m_{j2}\rangle \quad -(19)$$

where the C symbols are the Clebsch - Gordan coefficients also known as the Wigner coefficients or 3j symbols.

For the $m_s = 0$ state

$$|\tfrac{1}{2}, \tfrac{1}{2} ; 1, 0\rangle = C_{\frac{1}{2}, -\frac{1}{2}} \alpha_1 \beta_2 + C_{-\frac{1}{2}, \frac{1}{2}} \beta_1 \alpha_2 \quad -(20)$$

Clebsch Gordan Coefficients for $s_1 = \frac{1}{2}$, $s_2 = \frac{1}{2}$

m_{s1}	m_{s2}	$\|1,1\rangle$	$\|1,0\rangle$	$\|0,0\rangle$	$\|1,-1\rangle$
$\frac{1}{2}$	$\frac{1}{2}$	1	0	0	0
$\frac{1}{2}$	$-\frac{1}{2}$	0	$\left(\frac{1}{2}\right)^{1/2}$	$\left(\frac{1}{2}\right)^{1/2}$	0
$-\frac{1}{2}$	$\frac{1}{2}$	0	$\left(\frac{1}{2}\right)^{1/2}$	$-\left(\frac{1}{2}\right)^{1/2}$	0
$-\frac{1}{2}$	$-\frac{1}{2}$	0	0	0	1

Para Positronium

$$\boxed{|1,1\rangle := |\tfrac{1}{2}, \tfrac{1}{2} ; \tfrac{1}{2}, \tfrac{1}{2}\rangle = |\tfrac{1}{2}, \tfrac{1}{2} ; 1, 1\rangle = \alpha_1 \alpha_2 \quad -(21)}$$

5) <u>Ortho Positronium</u>

$$|1,0\rangle = \left(\frac{1}{2}\right)^{1/2}(\alpha_1\beta_2 + \beta_1\alpha_2) \quad -(22)$$

$$|1,-1\rangle = \beta_1\beta_2 \quad -(23)$$

$$|0,0\rangle = \left(\frac{1}{2}\right)^{1/2}(\alpha_1\beta_2 - \beta_1\alpha_2) \quad -(24)$$

<u>Pauli Exclusion Principle</u>

From eqs. (22) and (24) it is seen that:

$$\boxed{\text{SPATIAL}} : \phi_{\pm}(1,2) = \left(\frac{1}{2}\right)^{1/2}\left(a(1)b(2) \pm b(1)a(2)\right) \quad -(25)$$

where

$$a(1) = \phi_{n_1 l_1 m_{l_1}} \text{ (electron)}$$

$$b(2) = \phi_{n_2 l_2 m_{l_2}} \text{ (positron)}$$

$$b(1) = \phi_{n_1 l_1 m_{l_1}} \text{ (positron)}$$

$$a(2) = \phi_{n_2 l_2 m_{l_2}} \text{ (electron)}$$

If $$n = n_1 = n_2 \quad -(26)$$

then eq. (25) is the same as eqs. (22) and (24).

If the electron is at $\underline{r_1}$ and the positron is

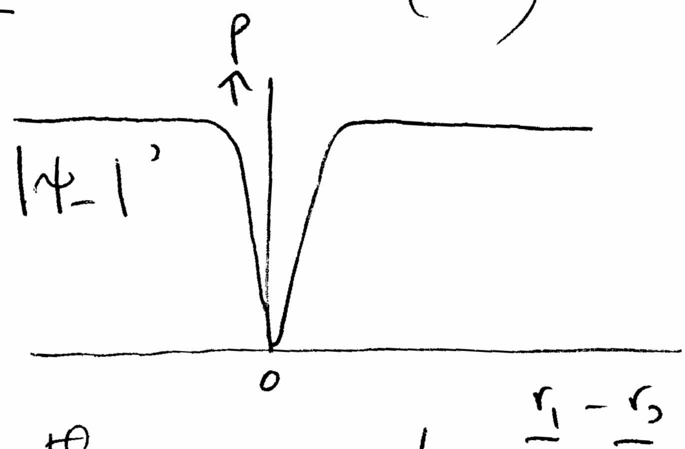
6)

at $\underline{r_2}$ then:

$$\phi_{\pm}(\underline{r_1}, \underline{r_2}) = \left(\frac{1}{2}\right)^{1/2} \left(\alpha_1(\underline{r_1})\beta_2(\underline{r_2}) \pm \alpha_2(\underline{r_1})\beta_1(\underline{r_2})\right) \quad -(25)$$

The amplitude of the function ϕ_- vanishes when:

$$\underline{r_1} = \underline{r_2}. \quad -(26)$$



This means that there is zero probability of finding both the electron and positron at the same point in space if they occupy ϕ_-.

The exchange integral is defined as:

$$K = \frac{e^2}{4\pi\epsilon_0} \int \left(a(1)b(1)\right) \frac{1}{r_{12}} \left(a(2)b(2)\right) d\tau_1 d\tau_2 \quad -(27)$$

This is a purely quantum result and does not depend on charge, or on the fact that the positron has a positive charge and electron has a negative charge.

The Pauli exclusion principle states that the total wavefunction (including spin) must be antisymmetric with respect to any pair of fermions. So the only allowed states are:

$$\psi = \begin{cases} \phi_+(1,2)(\alpha_1\beta_2 - \beta_1\alpha_2) \\ \phi_-(1,2)\,\alpha_1\alpha_2 \\ \phi_-(1,2)(\alpha_1\beta_2 + \beta_1\alpha_2) \\ \phi_-(1,2)\,\beta_1\beta_2 \end{cases} \qquad -(28)$$

The Schrödinger equation of positronium is therefore:

$$H\phi = E\phi \qquad -(29)$$

where

$$H = -\frac{\hbar^2\nabla^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r_{12}} \qquad -(30)$$

The Pauli exclusion principle does not depend on electric charge, and can be derived from rotation operators alone. So it applies to positronium. This means that the electron and positron in positronium cannot have the same set of quantum numbers. For a given principal quantum number n and orbital angular momentum quantum number l, the electron and positron cannot have the same spin quantum number, s.

8)

If the spin state of the electron and positron were the same, their joint state is $\alpha_1 \alpha_2$, which is symmetric:

$$\alpha_1 \alpha_2 = \alpha_2 \alpha_1 \quad \text{— (31)}$$

The Pauli principle states that the corresponding spatial part of the wave function must be antisymmetric and of the type $a(1)\,b(2) - b(1)\,a(2)$. If a is the same orbital as b then amplitude is zero for all r_1 and r_2. Therefore the amplitude of the state for an electron and positron with the same spin in the same orbital is identically zero. No such state exists. In order for such a state to exist, the electron and positron must have opposite spins..

Ground State of Positronium (Para, opposite spins)

The total wave function is:

$$\boxed{\phi(1,2) = \phi_{1s}(r_1)\,\phi_{1s}(r_2)\left(\frac{1}{2}\right)^{1/2}\left(\alpha_1\beta_2 - \beta_1\alpha_2\right)} \quad \text{— (32)}$$

$$= \left(\frac{1}{2}\right)^{1/2} \begin{vmatrix} \phi_{1s}(r_1)\,\alpha_1 & \phi_{1s}(r_1)\,\beta_1 \\ \phi_{1s}(r_2)\,\alpha_2 & \phi_{1s}(r_2)\,\beta_2 \end{vmatrix}$$

The spin-orbital is defined as:

i)

$$\psi_{1s}^{\alpha}(1) := \psi_{1s}(\underline{r}_1)\,\alpha_1 \quad -(33)$$

$$\psi_{1s}^{\beta}(1) := \psi_{1s}(\underline{r}_1)\,\beta_1 \quad -(34)$$

The Slater determinant is ~~then~~:

$$\psi(1,2) = \left(\frac{1}{2}\right)^{1/2} \begin{vmatrix} \psi_{1s}^{\alpha}(1) & \psi_{1s}^{\beta}(1) \\ \psi_{1s}^{\alpha}(2) & \psi_{1s}^{\beta}(2) \end{vmatrix} \quad -(35)$$

and

$$\boxed{\psi_{para}^{1s}(1,2) = -\psi_{para}^{1s}(2,1)} \quad -(36)$$

in accordance with the Pauli exclusion principle.

Ground State of Positronium (ortho, same spins)

In this case:

$$\psi_{ortho}(1,2) = \left(\frac{1}{2}\right)^{1/2} \begin{vmatrix} \psi_{1s}^{\alpha}(1) & \psi_{1s}^{\alpha}(1) \\ \psi_{1s}^{\alpha}(2) & \psi_{1s}^{\alpha}(2) \end{vmatrix} \quad -(37)$$

$$\boxed{\psi_{ortho}^{1s}(1,2) = 0.}$$

Therefore there is no ground state of ortho positronium from the Schrodinger equation.

10)

Total Wave functions of Ortho Positronium

These are:

$$\left.\begin{aligned} \phi &= \phi_-(1,2)\,\alpha_1\alpha_2 \\ &\phi_-(1,2)\,(\alpha_1\beta_2+\beta_1\alpha_2) \\ &\phi_-(1,2)\,\beta_1\beta_2 \end{aligned}\right\} \quad -(38)$$

where:

$$\phi_-(1,2) = \left(\frac{1}{2}\right)^{1/2}\left(a(1)b(2) - b(1)a(2)\right) \quad -(39)$$

and

$$a(1) = \phi_{n_1 l_1 m_{l_1}} \quad (\text{electron})$$

$$b(2) = \phi_{n_2 l_2 m_{l_2}} \quad (\text{positron})$$

$$b(1) = \phi_{n_1 l_1 m_{l_1}} \quad (\text{positron})$$

$$a(2) = \phi_{n_2 l_2 m_{l_2}} \quad (\text{electron})$$

$$\alpha_1\alpha_2 = \left|\tfrac{1}{2},\tfrac{1}{2};\tfrac{1}{2},\tfrac{1}{2}\right\rangle = |1,1\rangle$$

$$\alpha_1\beta_2 = \left|\tfrac{1}{2},\tfrac{1}{2};\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = |1,0\rangle$$

$$\beta_1\alpha_2 = \left|\tfrac{1}{2},-\tfrac{1}{2};\tfrac{1}{2},\tfrac{1}{2}\right\rangle = |1,-1\rangle$$

$$\beta_1\beta_2 = \left|\tfrac{1}{2},-\tfrac{1}{2};\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = |0,0\rangle$$

11) The total angular momentum state is made up of $|s_1 m_{s1}; s_2 m_{s2}\rangle$ with:

$$m_{s1} = \pm\frac{1}{2},\ m_{s2} = \pm\frac{1}{2} \quad -(40)$$

It is seen that the electron and positron cannot occupy the same spatial orbital, i.e.

$$a(1)b(2) \neq b(1)a(2) \quad -(41)$$

otherwise:

$$\phi_-(1,2) = 0 \quad -(42)$$

The Schrödinger equation is:

$$\boxed{H\phi_-(1,2) = E\phi_-(1,2)} \quad -(43)$$

which describes an electron bound to a positron through a Coulomb Law:

$$V = -\frac{e^2}{4\pi\epsilon_0 r_{12}} \quad -(43)$$

where:

$$r_{12} = |\underline{r}_1 - \underline{r}_2|. \quad -(44)$$

This produces H-like solutions, but with added features as described. There cannot be a ground state of ortho-positronium because $n_1 = n_2 = n = 1,\ l = 0,$ and

12)

$$\psi_-(n_1 = n_2 = 1, \ell = 0) = 0 \quad -(45)$$

States of Ortho Positronium

These are determined by equation (41). So there can be a state, for example:

Electron	Positron
$n_1 = 2, \ell_1 = 0$	$n_2 = 1, \ell_2 = 0$

So:

$$a(1) = \psi_{20}\ (\text{electron})$$
$$b(2) = \psi_{10}\ (\text{positron})$$
$$b(1) = \psi_{20}\ (\text{positron})$$
$$a(2) = \psi_{10}\ (\text{electron})$$

and:

$$\psi_-(1,2) = \left(\frac{1}{2}\right)^{1/2}\left(a(1)b(2) - b(1)a(2)\right)$$
$$\neq 0.$$

Here:

$$a(2) = \psi_{10}\ (\text{electron}) = \exp\left(-\frac{r_1}{a}\right)$$
$$b(2) = \psi_{10}\ (\text{positron}) = \exp\left(-\frac{r_2}{a}\right)$$
$$a(1) = \psi_{20}\ (\text{electron}) = \left(2 - \frac{r_1}{a}\right)\exp\left(-\frac{r_1}{2a}\right)$$
$$b(1) = \psi_{20}\ (\text{positron}) = \left(2 - \frac{r_2}{a}\right)\exp\left(-\frac{r_2}{2a}\right)$$

13)

$$\boxed{\psi_-(1,2) = \left(\frac{1}{2}\right)^{1/2}\left(e^{-r_2/a}\left(2-\frac{r_1}{a}\right)e^{-r_1/(2a)} - e^{-r_1/a}\left(2-\frac{r_2}{a}\right)e^{-r_2/(2a)}\right)} \quad -(46)$$

Therefore for $\psi_1(1,2)$ to exist:

$$r_1 \neq r_2 \quad -(47)$$

The total wave functions are ~~therefore~~:

$$\psi = \psi_-(1,2)\,|1,1\rangle$$
$$= \psi_-(1,2)\left(|1,0\rangle + |1,-1\rangle\right)$$
$$= \psi_-(1,2)\,|0,0\rangle \quad -(48)$$

with $\psi_-(1,2)$ given by equation (46)

If the electron and positron are at the same point in space:

$$\underline{r_1} = \underline{r_2} \quad -(49)$$

14) ~~the~~ :

$$\phi = 0 \quad -(50)$$

and ~~the~~ ortho positronium cannot exist.

The decay properties of para and ortho positronium depend on ~~the~~ nature of $\phi_-(1,2)$ and $\phi_+(1,2)$. In para, ~~when~~ at ~~the~~ electron and positron may exist

$$r_1 = r_2 \quad -(51)$$

but not in ortho.