Problem 1. Positronium is a hydrogen-like atom in which the proton (nucleus) is replaced with a positron. While this system is unstable against electron–positron annihilation, it lives long enough to detect it and study its properties.

(a) What is the wavelength of the transition between the ground and first excited state (analogue of the Lyman-alpha line in hydrogen) in positronium? Give your answer in nanometers.

(b) What is the most probable distance between the positron and electron in the ground state of positronium? Give your answer in meters or Angstroms.

(c) The annihilation rate in positronium, Γ, ($\Gamma = 1/\tau$, where τ is the lifetime) is proportional to the probability that the positron and electron happen to be in (nearly) the same point in space. Suppose we know the lifetime of positronium in the ground state, τ_0. What is the lifetime of positronium in the first excited state then? Note that the first excited state is degenerate and each state from that degenerate multiplet may have a different lifetime. Ignore the fact that the particles have spin.

Solution:

The reduced mass in this hydrogen-like atom (denoted Ps), is $\mu = \frac{m_1 m_2}{m_1+m_2} = \frac{m_e m_e}{m_e+m_e} = \frac{m_e}{2}$. This value of the reduced mass should be put in all relevant expressions that contain μ.

(a) For the energy levels we have

$$E_n = -\frac{\mu e^4}{32\pi^2\hbar^2\epsilon_0^2}\frac{1}{n^2}.$$

The energy difference between states $n = 2$ and $n = 1$ is then

$$\Delta E_{21} = \frac{3\mu e^4}{128\pi^2\hbar^2\epsilon_0^2} = \frac{3m_e e^4}{64h^2\epsilon_0^2}.$$

The transition wavelength is

$$\lambda_{21} = \frac{hc}{\Delta E_{21}} = \frac{64h^3\epsilon_0^2 c}{3m_e e^4} \approx 243\,\text{nm}.$$

This wavelength for Ps atom is roughly twice longer than the corresponding one for the common hydrogen atom, ^{1}H.

(b) The probability density distribution in the ground state of a hydrogen-like atom is given by

$$\rho(r) = 4\pi r^2|\psi_{100}(r)| = r^2|R_{10}(r)|^2,$$

where r^2 comes from the Jacobian in the spherical coordinates. R_{10} is the radial wave function,

$$R_{10}(r) = \frac{2}{a^{3/2}}\, e^{-\frac{r}{a}}.$$

In the latter expression a is the Bohr radius for Ps, $a = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2} = \frac{8\pi\epsilon_0\hbar^2}{m_e e^2}$, which is twice larger than that for ^{1}H.

The most probable distance between the electron and positron corresponds to the maximum of the density distribution function $\rho(r)$:

$$\rho(r) \propto r^2 e^{-\frac{2r}{a}}, \qquad \left(2r_{\max} - \frac{2r_{\max}^2}{a}\right) e^{-\frac{2r_{\max}}{a}} = 0,$$

$$r_{\max} = a \approx 1.058\times 10^{-10}\ \mathrm{m} = 1.058\ \mathrm{Angstrom}.$$

(c) The positron and electron happen to be in the same point in space when the distance between them is zero, i.e. $r = 0$. The annihilation rate is then proportional to $\rho(r=0) = |\psi(r=0)|^2$. Hence,

$$\frac{\Gamma_{\mathrm{gr}}}{\Gamma_{\mathrm{ex}}} = \frac{|\psi_{\mathrm{gr}}(0)|^2}{|\psi_{\mathrm{ex}}(0)|^2}, \qquad \text{or} \qquad \tau_{\mathrm{ex}} = \frac{|\psi_{\mathrm{gr}}(0)|^2}{|\psi_{\mathrm{ex}}(0)|^2}\,\tau_{\mathrm{gr}}\,.$$

The excited state ($n = 2$) is four-fold degenerate. The multiplet contains the following states ψ_{nlm}:

$$\psi_{200},\ \psi_{211},\ \psi_{210},\ \psi_{21-1}.$$

The wave functions corresponding to $l = 1$ quantum number, namely ψ_{211}, ψ_{210}, and ψ_{21-1} all vanish at $r = 0$. Therefore, Ps lifetime in those states will be infinite, $\tau_{\mathrm{ex}} = \infty$ (in reality the system will first decay to the ground state and then annihilate there). However, for state ψ_{200} we have

$$\tau_{\mathrm{ex}} = \frac{|R_{10}(0)|^2}{|R_{20}(0)|^2}\,\tau_{\mathrm{gr}} = \frac{|2a^{-3/2}|^2}{\left|\frac{1}{\sqrt{2}}a^{-3/2}\right|^2}\,\tau_{\mathrm{gr}} = 8\tau_{\mathrm{gr}}\,.$$

Problem 2. The total wave function, which depends on both spatial (r, θ, ϕ) and spin variables, of an electron in the hydrogen atom is given by the following expression:

$$\Psi = A \begin{pmatrix} \sin\phi \, \sin\theta \, \frac{r}{a_0} \exp\left[-\frac{r}{2a_0}\right] \\ 2\exp\left[-\frac{r}{a_0}\right] \end{pmatrix},$$

Here A is a normalization constant and a_0 is the Bohr radius. What values and with what probabilities will be obtained if we measure

(a) Energy

(b) Square of the orbital angular momentum

(c) Projection of the orbital angular momentum on the z-axis

(d) Projection of the spin on the z-axis

(e) Projection of the total angular momentum (orbital ang. mom. + spin) on the z-axis

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Solution:

In the most general case of Ψ we would need to expand it in terms of the hydrogenic wave functions multiplied by spin-up or spin-down states. That would amount to taking integrals in 3D, which might not be trivial to compute. However, in our case Ψ has a simple form that can be easily expressed in terms of of the hydrogenic states. Note that

$$R_{10}(r) = \frac{2}{a_0^{3/2}} \exp\left[-\frac{r}{a_0}\right], \qquad R_{21}(r) = \frac{1}{\sqrt{24}\, a_0^{3/2}} \frac{r}{a_0} \exp\left[-\frac{r}{2a_0}\right],$$

$$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}}, \qquad Y_1^1(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin\theta\, e^{i\phi}, \qquad Y_1^{-1}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin\theta\, e^{-i\phi},$$

and

$$\sin\theta\, \sin\phi = i\sqrt{\frac{2\pi}{3}}(Y_1^1 + Y_1^{-1}).$$

With that our total wave function can be written as

$$\Psi = A \begin{pmatrix} i\sqrt{\frac{2\pi}{3}}\,(Y_1^1 + Y_1^{-1})\sqrt{24}\, a^{3/2} R_{21} \\ 2\sqrt{4\pi}\, Y_0^0 \frac{1}{2}\, a^{3/2} R_{10} \end{pmatrix} = A a^{3/2} \begin{pmatrix} i\sqrt{16\pi}\,(Y_1^1 + Y_1^{-1}) R_{21} \\ \sqrt{4\pi}\, Y_0^0 R_{10} \end{pmatrix},$$

or simply

$$\Psi = A a^{3/2}\left[4i\sqrt{\pi}\, Y_1^1 R_{21}\chi_+ + 4i\sqrt{\pi}\, Y_1^{-1} 1 R_{21}\chi_+ + 2\sqrt{\pi}\, Y_0^0 R_{10}\chi_-\right],$$

where $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ are spin-up and spin-down states respectively. Given that the spherical harmonics, radial hydrogenic wave functions, and spin states $\chi_\pm$ are normalized, we can easily determine constant A, which yields:

$$\Psi = \frac{2i}{3} Y_1^1 R_{21}\chi_+ + \frac{2i}{3} Y_1^{-1} R_{21}\chi_+ + \frac{1}{3} Y_0^0 R_{10}\chi_- = \frac{2i}{3}\psi_{211}\chi_+ + \frac{2i}{3}\psi_{21-1}\chi_+ + \frac{1}{3}\psi_{100}\chi_-\,.$$

In the above expression $\psi_{nlm}(r,\theta,\phi)$ stands for the hydrogenic wave functions corresponding to quantum numbers n, l, and m. It can be seen that the probability of finding the system in state $\psi_{211}\chi_+$ is $P_{211\uparrow} = 4/9$, in state $\psi_{21-1}\chi_+$ is $P_{21-1\uparrow} = 4/9$, and in state $\psi_{100}\chi_-$ is $P_{100\downarrow} = 1/9$. The probability of finding the system in any other state is zero. Based on this we can answer questions (a)-(e):

(a) Possible values of energy:

$$1)\ E_1 = -\frac{m_e}{2\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2 = -\frac{1}{2}\ \text{hartree} \qquad P(E_1) = P_{100\downarrow} = \frac{1}{9}$$

$$2)\ E_2 = -\frac{m_e}{8\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2 = -\frac{1}{8}\ \text{hartree} \qquad P(E_1) = P_{211\uparrow} + P_{21-1\uparrow} = \frac{8}{9}.$$

(b) Possible values of the square of the orbital angular momentum:

$$1)\quad 0 \qquad P(0) = P_{100\downarrow} = \frac{1}{9},$$

$$2)\ \hbar^2 1(1+1) = 2\hbar^2 \qquad P(2\hbar^2) = P_{211\uparrow} + P_{21-1\uparrow} = \frac{8}{9}.$$

(c) Possible values of the projection of the orbital angular momentum on the z-axis:

$$1)\quad 0 \qquad P(0) = P_{100\downarrow} = \frac{1}{9},$$

$$2)\ +\hbar \qquad P(+\hbar) = P_{211\uparrow} = \frac{4}{9},$$

$$3)\ -\hbar \qquad P(-\hbar) = P_{21-1\uparrow} = \frac{4}{9}.$$

(d) Possible values of the projection of the spin on the z-axis:

$$1)\ +\frac{\hbar}{2} \qquad P(+\hbar/2) = P_{211\uparrow} + P_{21-1\uparrow} = \frac{8}{9},$$

$$2)\ -\frac{\hbar}{2} \qquad P(-\hbar/2) = P_{100\downarrow} = \frac{1}{9}.$$

(e) Possible values of the projection of the total angular momentum (the sum of orbital angular momentum and spin) on the z-axis:

$$1)\ +\frac{3\hbar}{2} \qquad P(+3\hbar/2) = P_{211\uparrow} = \frac{4}{9},$$

$$2)\ -\frac{\hbar}{2} \qquad P(-\hbar/2) = P_{21-1\uparrow} + P_{100\downarrow} = \frac{5}{9}.$$

Problem 3. Consider an electron in the state corresponding to the positive projection of its spin on the z axis. Now we measure the projection of the spin on axis z', which makes angle θ with z. What are the probabilities of getting the positive and negative values?

Solution:

The state corresponding to the positive projection of spin on the z axis is an eigenstate of $S_z = \frac{\hbar}{2}\sigma_z$:

$$|\chi_+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

There are many possible choices for a z' axis that makes angle θ with axis z. Most generally, we can define a unit vector $\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\cos\phi, \cos\theta)$. However, due to the symmetry of the problem we can pick any specific value of ϕ. For simplicity, let us use $\phi = 0$. Then $\mathbf{n} = (\sin\theta,\, 0,\, \cos\theta)$. The operator corresponding to the projection of spin on axis z' defined by unit vector $\mathbf{n}$ is:

$$\mathbf{n}\cdot\mathbf{S} = \frac{\hbar}{2}\mathbf{n}\cdot\boldsymbol{\sigma} = \frac{\hbar}{2}(\sigma_x\sin\theta + \sigma_z\cos\theta),$$

or, in matrix form,

$$\frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}.$$

The eigenvalues and the corresponding normalized eigenvectors of this 2×2 matrix are

$$\lambda_+ = +\frac{\hbar}{2}, \qquad |\eta_+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix},$$

$$\lambda_- = -\frac{\hbar}{2}, \qquad |\eta_-\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}.$$

The expansion of state $|\chi_+\rangle$ in terms of $|\eta_+\rangle$ and $|\eta_-\rangle$ (which form a complete basis) is

$$|\chi_+\rangle = |\eta_+\rangle \underbrace{\langle\eta_+|\chi_+\rangle}_{c_+} + |\eta_-\rangle \underbrace{\langle\eta_-|\chi_+\rangle}_{c_-}.$$

Absolute squares of coefficients $c_+ = \cos\frac{\theta}{2}$ and $c_- = \sin\frac{\theta}{2}$ give the probabilities of finding the system in states $|\chi_+\rangle$ and $|\chi_-\rangle$ respectively. Therefore, the probabilities of getting the positive and negative values when the projection of the spin on axis z' is measured are

$$P_+ = \cos^2\frac{\theta}{2},$$

$$P_- = \sin^2\frac{\theta}{2}.$$