LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Quantum Physics MTF107

Examination date: 2008-08-30
Note solutions are more detailed compared to previous solutions, earlier than October 2007.

1. The relevant radial part of the wave function is: $R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}$. The probability to find the particle in the range r och $r+dr$ is given by: $P(r)dr = R_{21}(r)^2r^2dr$ and hence $P(r) = R_{21}(r)^2r^2 = \text{konstant } r^4e^{-Zr/a_0}$.

   The extreme is where the derivative is zero.
   $\frac{dP(r)}{dr} = 4r^3e^{-Zr/a_0} - r^4\frac{Z}{a_0}e^{-Zr/a_0} = r^3(4 - r\frac{Z}{a_0})e^{-Zr/a_0} = 0$. The maximum appears at $r = 4a_0$. It is a maximum as $P(0) = P(\infty) = 0$ and $P(r) \geq 0$ and hence a maximum. You can also study the sign change of the derivative to the left and right of the extremum or you can investigate the sign of the second derivative at the extreme.

   If there are no external electric or magnetic fields the energy of the hydrogenic levels depends only on the principal quantum number n and not on the angular momentum quantum numbers l and m_l.

   For this case the following states have the same energy:
   I) 3s with $m_l = 0$, 3p with $m_l = 1$, 3p with $m_l = -1$, 3p with $m_l = 0$.
   II) 4d with $m_l = 1$, 4p with $m_l = 0$, 4p with $m_l = -1$.
   III) 5d with $m_l = 1$, 5p with $m_l = -1$, 5s with $m_l = 0$.

2. The eigenfunctions of the infinite square well in one dimension are (Here a solution of the S.E. in one dimension is adequate). The width of the well is a.

   $$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \quad \text{and the eigenenergys are } E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad \text{where} \quad n = 1, 2, 3, ...$$

   In three dimensions the eigenfunctions and eigenenergys are (Here an argument about separation of variables is needed to justify the structure of the solution)

   $\Psi_{n,m,l}(x, y) = \psi_n(x)\cdot\psi_m(y)\cdot\psi_l(z)$ and eigenenergys $E_{n,m} = E_n + E_m + E_l$ where the indecies are $n = 1, 2, 3, ..$, $m = 1, 2, 3, ..$ and $l = 1, 2, 3, ..$

   a) The eigenfunctions inside the box are (note the side length is $a/2$ for one of the sides)

   $$\Psi_{n,m,l}(x, y, z) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\cdot\sqrt{\frac{2}{a}}\sin\frac{m\pi y}{a}\cdot\sqrt{\frac{4}{a}}\sin\frac{l\pi 2y}{a} \quad \text{where} \quad n = 1, 2, 3, .. , m = 1, 2, 3, .. \text{ and } \quad l = 1, 2, 3,$$

   The eigenfunctions outside the box are $\Psi_{n,m,l}(x, y, z) = 0$
   b) The six lowest eigenenergys are

   $$E_{n,m,l} = \frac{\pi^2\hbar^2}{2ma^2}(n^2 + m^2 + 4l^2), \quad \text{where the 5 lowest are} \quad (n^2 + m^2 + 4l^2) = 6, 9, 12, 14, 18, \text{ and } 21.$$

   c) The six lowest eigenenergys have degeneracys (either one, two or four) as follows:

   $$E_{1,1,1} = \text{ one state } \ (n^2 + m^2 + 4l^2 = 6)$$

   $$E_{1,2,1} = E_{2,1,1} = \text{ two states } \ (n^2 + m^2 + 4l^2 = 9)$$

$$
\begin{aligned}
E_{2,2,1} = & \text{ one state } \ (n^2+m^2+4l^2=12)\\
E_{1,3,1} = E_{3,1,1} = & \text{ two states } \ (n^2+m^2+4l^2=14)\\
E_{2,3,1} = E_{3,2,1} = & \text{ two states } \ (n^2+m^2+4l^2=17)\\
E_{1,1,2} = & \text{ one state } \ (n^2+m^2+4l^2=18)
\end{aligned}
$$

Energy number 7 is special as the degeneracy is 4 but all four are not connected through a symmetry operation, ie some of these states are accidentally degenerated. These four can be grouped in the following way.

$$E_{1,2,2} = E_{2,1,2} = \text{ two states } \ (n^2+m^2+4l^2=21)$$

$$E_{1,4,1} = E_{4,1,1} = \text{ two states } \ (n^2+m^2+4l^2=21)$$

3. **a**

The spinor is not normalised and we need to do this first:

$$1 = \chi^*\chi =\mid A\mid^2 (2-5i, 3+i)\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} =\mid A \mid^2 \mid 2+5i\mid^2 \mid 3-i\mid^2 \rightarrow \ A = \frac{1}{\sqrt{39}}$$

Note an expectation value is always a real number, never a complex one! Even if you had taken A to be a complex number like $A = \frac{i}{\sqrt{39}}$ it would not change the expectation value as the expectation value below only involves $\mid A\mid^2$.

$$< S_x >= \frac{1}{39}(2-5i, 3+i)\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \frac{1}{39}\hbar$$

$$< S_y >= \frac{1}{39}(2-5i, 3+i)\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = -\frac{17}{39}\hbar$$

$$< S_z >= \frac{1}{39}(2-5i, 3+i)\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \frac{19}{78}\hbar$$

b

Measurement along the x direction means: $S = (1,0,0)\cdot(S_x, S_y, S_z) = S_x$. The idea is to expand the initial spinor χ into the eigenspinors of S_x. So we start to calculate the eigenvalues and eigenspinors to S_x. The spin operator S_x is

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

we find the eigenvalues from the following equation

$$S_n\chi = \lambda\chi \Leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix} \tag{1}$$

We find the eigenvalues from the equation

$$\begin{vmatrix} -\lambda & 1\frac{\hbar}{2} \\ 1\frac{\hbar}{2} & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm\frac{\hbar}{2}$$

The eigenspinors to S_x corresponding to the $+\frac{\hbar}{2}$ we get from

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = +\frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}$$

The two equations above are linearly dependent and one of them is

$$a = b \Leftrightarrow \text{ let } \ b = 1 \ \text{ and hence } \ a = 1$$

This gives the unnormalised spinor

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and after normalisation we have } \ \chi_{x+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

The other eigenspinor χ_{x-} has to be orthogonal to χ_{x+}. An appropriate choice is:

$$\chi_{x-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Now we can expand the initial spinor χ in these eigenspinors to S_x. the second eigenspinor you can get from orthogonality to the first one.

$$\chi = \frac{1}{\sqrt{39}}\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = b_+\chi_{x+} + b_-\chi_{x-}$$

The coefficient b_+ is given by

$$b_+ = \chi_{x+}^*\chi = \frac{1}{\sqrt{78}}(1 \quad 1) * \begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \frac{1}{\sqrt{78}}(2+5i+3-i) = \frac{1}{\sqrt{78}}(5+4i)$$

A similar calculation gives b_- :

$$b_+ = \chi_{x+}^*\chi = \frac{1}{\sqrt{78}}(1 \quad -1) * \begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \frac{1}{\sqrt{78}}(2+5i-3+i) = \frac{1}{\sqrt{78}}(-1+6i)$$

We may now check that $\mid b_+ \mid^2 + \mid b_- \mid^2 = 1$

$$\mid b_+ \mid^2 + \mid b_- \mid^2 = \frac{1}{78}(25+16+1+36) = 1 \quad \text{ok}$$

The probability (to get $+\frac{\hbar}{2}$) is given by $|b_+|^2$.

$$|b_+|^2 = \frac{1}{78}(25+16) = \frac{41}{78} \approx \mathbf{0.526}$$

and (to get $-\frac{\hbar}{2}$) is given by $|b_-|^2$.

$$|b_-|^2 = \frac{1}{78}(1+36) = \frac{37}{78} \approx \mathbf{0.474}$$

You may make the following check for consistency:

$$< S_x > = \left(\frac{41}{78}(\frac{\hbar}{2}) + \frac{37}{78}(-\frac{\hbar}{2})\right) = \frac{1}{39}\hbar$$

The same result as in part **a**.

4. Rewrite the wave function in terms of spherical harmonics: (polar coordinates: $x = r\sin\theta\sin\phi$, $z = r\cos\theta$ and hence $zx = r^2\cos\theta\sin\theta(e^{i\phi}+e^{-i\phi})/2$ using the Euler relations) the appropriate spherical harmonics can now be identified and we arrive at

$$\psi(\boldsymbol{r}) = \psi(x,y,z) = N(zx)e^{-r/3a_0} = N\frac{r^2}{2}\sqrt{\frac{8\pi}{15}}(-Y_{2,1}+Y_{2,-1})e^{-r/3a_0} \ . \qquad (2)$$

As all the involved $Y_{l,m}$ have $l = 2$ the probability to get $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$ is one. For the operator L_z we note the two spherical harmonics have the same pre factor (one has -1 and the other has +1 but the absolute value square is the same) ie they will have the same probability. The probability to find $m = 2\hbar$ is 0, for $m = 1\hbar$ is $\frac{1}{2}$, for $m = 0\hbar$ is 0 for $m = -1\hbar$ is $\frac{1}{2}$, and for $m = -2\hbar$ is 0. As all the involved $Y_{l,m}$ have $l = 2$ the probability to get $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$ is one.

b. To calculate the expectation value $<r>$ we need to normalise the given wave function if we wish to do the integral. In order to achieve this in a simple way is to identify the radial wave function. As l is equal to 2 we now that n cannot be equal to 1 or 2 it has to be **larger** or **equal** to 3. By inspection of eq (2) and 2 we find $n = 3$ this function has the correct exponential and the correct power of r (r^2) and hence $R_{3,2}(r) = \frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Z}{3a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$. We also note that $Y_{2,1}$ and $Y_{2,-1}$ are normalised but the sum $(-Y_{2,1}+Y_{2,-1})$ is not normalised. The sum has to be changed to $(-\frac{1}{\sqrt{2}}Y_{2,1}+\frac{1}{\sqrt{2}}Y_{2,-1})$ in order to be normalised. Note that $R_{3,2}(r)$ contains an r^2 term as also a $e^{-r/3a_0}$ term. The wave function can now be completed to the following normalized wave function (note that we do not need to calculate the constant N as all separate parts of $\psi(r)$ are normalised by them selves)

$$\psi(\boldsymbol{r}) = \psi(x,y,z) = N(zx)e^{-r/3a_0} = R_{3,2}(r)(-\frac{1}{\sqrt{2}}Y_{2,1}+\frac{1}{\sqrt{2}}Y_{2,-1})e^{-r/3a_0}$$

From physics handbook page 292 you find

$$\langle r\rangle = \frac{1}{2}\left[3n^2 - l(l+1)\right]\left(\frac{a_0}{Z}\right) = \frac{1}{2}\left[3\ 3^2 - 2(2+1)\right]\left(\frac{a_0}{1}\right) = \frac{21}{2}a_0 =$$

$$10.5\ \cdot 0.5292\ \text{Å} = 5.56\ \text{Å}.$$

You may also do the integral directly like this:

$$\langle r\rangle = \int_0^\infty\int_0^\pi\int_0^{2\pi} d\phi\ d\theta\ dr\ r^2\sin(\theta)\ r\ \mid R_{3,2}(r)\mid^2 \mid\left(-\frac{1}{\sqrt{2}}Y_{2,1}+\frac{1}{\sqrt{2}}Y_{2,-1}\right)\mid^2\ e^{-2r/3a_0} =$$

$$\int_0^\infty dr\ r^3 \mid R_{3,2}(r)\mid^2 e^{-2r/3a_0} = \frac{21}{2}a_0 = 10.5\ \cdot 0.5292\ \text{Å} = 5.56\ \text{Å}.$$

5. (a) $\langle H\rangle = \frac{1}{2}0.27 + \frac{1}{4}1.08 + \frac{3}{16}3.65 + \frac{1}{16}4.06 = 1.343125 \approx 1.34\text{eV}$.
   Uncertainty is defined by: $\langle\Delta H\rangle = \sqrt{\langle H^2\rangle - \langle H\rangle^2}$
   $\langle H^2\rangle = \frac{1}{2}(0.27)^2 + \frac{1}{4}(1.08)^2 + \frac{3}{16}(3.65)^2 + \frac{1}{16}(4.06)^2 = 3.85624375\ (\text{eV})^2$.
   $\langle\Delta H\rangle = \sqrt{3.85624375 - 1.343125^2} = 1.432571 \approx 1.43\text{eV}$

(b) The expression is not unique as we only know the probabilities which are the squares of the coefficients. In the evaluation of $\langle H \rangle$ and $\langle H^2 \rangle$ only the probabilities are important that's why a different sign $\pm$ is of no importance in this calculation.

One is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \frac{1}{2}\psi_2(z) + \frac{\sqrt{3}}{4}\psi_3(z) + \frac{1}{4}\psi_4(z)$.

Another is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) - \frac{1}{2}\psi_2(z) + \frac{\sqrt{3}}{4}\psi_3(z) - \frac{1}{4}\psi_4(z)$.