LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS F0047T

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The solutions are just suggestions. They may contain several alternative routes.

1. (a) $i\hbar\frac{\partial^2}{\partial t^2}\cos\omega t = -i\hbar\omega\frac{\partial}{\partial t}\sin\omega t = -i\hbar\omega^2\cos\omega t$ **YES**
   (b) $\frac{\partial}{\partial x}e^{ikx} = ike^{ikx}$ **YES**
   (c) $\frac{\partial}{\partial x}e^{-ax^2} = -2axe^{-ax^2}$ **NO**
   (d) $\frac{\partial}{\partial x}\cos kx = -k\sin kx$ **NO**
   (e) $\frac{\partial}{\partial x}kx = k$ **NO**
   (f) $\hat{P}\sin(kx) = \sin(-kx) = -\sin(kx)$ **YES**
   (g) $-i\hbar\frac{\partial}{\partial z}C(1+z^2) = -i\hbar C(0+2z)$ **NO**
   (h) $-\frac{\hbar}{2}\frac{\partial}{\partial z}Ce^{-3z} = -\frac{\hbar}{2}C(-3)e^{-3z} \;\propto\; \psi(z)$ **YES**
   (i) $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} =?$ This has to be done in some steps. Start by doing this derivative first: $-\frac{\partial^2}{\partial z^2}ze^{-\frac{1}{2}z^2} = -\frac{\partial}{\partial z}(e^{-\frac{1}{2}z^2} - z^2e^{-\frac{1}{2}z^2}) = -(-ze^{-\frac{1}{2}z^2} - 2ze^{-\frac{1}{2}z^2} + z^3e^{-\frac{1}{2}z^2}) = 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}$.
   Now you go back to the start: $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} = \frac{C}{2}(z^3e^{-\frac{1}{2}z^2} + 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}) = \frac{C}{2}(+3ze^{-\frac{1}{2}z^2}) = \propto\; \psi(z)$ **YES**

2. **a**

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

$$1 = \chi^*\chi = \mid A\mid^2 (2-5i, 3+i)\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \mid A\mid^2 \left(\mid 2+5i\mid^2 + \mid 3-i\mid^2\right) = \mid A\mid^2 (29+10)\,,$$

$$\text{and hence}: \; A = \frac{1}{\sqrt{39}}$$

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

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

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

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

This eigenspinor χ_{x-} is orthogonal to the eigenspinor χ_{x+}.

Now we can expand the initial spinor χ in these eigenspinors of S_x.

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

The coefficient b_+ is given by

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

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**.

3. Rewrite the wave function in terms of spherical harmonics: (polar coordinates: $x = r\sin\theta\sin\phi, y = r\sin\theta\cos\phi, z = r\cos\theta$ and hence $xy = r^2\sin^2\theta\sin\phi\cos\phi = r^2\sin^2\theta(e^{i2\phi} - e^{-i2\phi})/4i$ using the Euler relations) the appropriate spherical harmonics can now be identified $Y_{2,-2} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{-i2\phi}$ and $Y_{2,2} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{i2\phi}$ and we arrive at

$$\psi(\boldsymbol{r}) = \psi(x, y, z) = N \cdot xy \cdot e^{-r/3a_0} = N\frac{r^2}{4i}\sqrt{\frac{32\pi}{15}}(Y_{2,2} - Y_{2,-2})e^{-r/3a_0} \ . \tag{2}$$

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 $\frac{1}{2}$, for $m = 1\hbar$ is 0, for $m = 0\hbar$ is 0 for $m = -1\hbar$ is 0, and for $m = -2\hbar$ is $\frac{1}{2}$. 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.

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 know 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 $Y_{2,2}$ and $Y_{2,-2}$ are normalised but the sum $(Y_{2,2} - Y_{2,-2})$ is not normalised. As the normalisation integral will produce 1+1=2, the sum has to be changed to $(\frac{1}{\sqrt{2}}Y_{2,2} - \frac{1}{\sqrt{2}}Y_{2,-2})$ 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)

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

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 (only the part depending on r are of interest as the angular parts just will be the normalising integral):

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

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

4. (a) $\langle H\rangle = \frac{1}{2}0.25 + \frac{1}{4}0.95 + \frac{1}{6}2.12 + \frac{1}{24}3.23 + \frac{1}{24}4.79 = 1.05000 \approx 1.05\text{eV}$.
   Uncertainty is defined by: $\langle \Delta H\rangle = \sqrt{\langle H^2\rangle - \langle H\rangle^2}$
   $\langle H^2\rangle = \frac{1}{2}0.25^2 + \frac{1}{4}0.95^2 + \frac{1}{6}2.12^2 + \frac{1}{24}3.23^2 + \frac{1}{24}4.79^2 = 2.39665 \approx 2.40\text{eV}^2$.
   $\langle \Delta H\rangle = \sqrt{2.39665 - 1.05^2} = 1.1376 \approx 1.14\text{eV}$

   (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 thats why a different sign $\pm$ is of no importance in this calculation.
   One is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \sqrt{\frac{1}{4}}\psi_2(z) + \frac{1}{\sqrt{6}}\psi_3(z) + \frac{\sqrt{1}}{24}\psi_4(z) + \frac{1}{24}\psi_5(z)$.
   Another is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \sqrt{\frac{1}{4}}\psi_2(z) - \frac{1}{\sqrt{6}}\psi_3(z) - \frac{\sqrt{1}}{24}\psi_4(z) + \frac{1}{24}\psi_5(z)$.

   (c) It would be lowered by a factor of 9. (All eigenvalues change by a factor of 9)

5. Hydrogenic atoms have eigenfunctions $\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta,\varphi)$. Using the COLLECTION OF FORMULAE we find

$$\begin{aligned}
\psi_{100}(\boldsymbol{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0}\\
\psi_{200}(\boldsymbol{r}) &= \left(\frac{Z^3}{8\pi a_0^3}\right)^{1/2}\left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0}\\
\psi_{210}(\boldsymbol{r}) &= \left(\frac{Z^3}{32\pi a_0^3}\right)^{1/2}\frac{Zr}{a_0}\cos\theta e^{-Zr/2a_0}\\
\psi_{21\pm1}(\boldsymbol{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2}\frac{Zr}{8a_0}\sin\theta e^{\pm i\varphi} e^{-Zr/2a_0}
\end{aligned}$$

where a_0 is the Bohr radius. The β-decay instantaneously changes $Z = 1 \to Z = 2$. According to the expansion theorem, it is possible to express the wave function $u_i(\boldsymbol{r})$ before the decay as a linear combination of eigenfunctions $v_j(\boldsymbol{r})$ after the decay as

$$u_i(\boldsymbol{r}) = \sum_j a_j v_j(\boldsymbol{r})$$

where

$$a_j = \int v_j^*(\boldsymbol{r})u_i(\boldsymbol{r})d^3r.$$

The probability to find the electron in state j is given by $|a_j|^2$.

(a) Here $u_i = \psi_{100}(Z=1)$ and $v_j = \psi_{200}(Z=2)$. This gives

$$\begin{aligned} a &= \left(\frac{1}{\pi a_0^3}\right)^{1/2}\left(\frac{2^3}{8\pi a_0^3}\right)^{1/2}\int_0^\infty e^{-r/a_0}\left(1-\frac{2r}{2a_0}\right)e^{-2r/2a_0}4\pi r^2 dr \\ &= \frac{4}{a_0^3}\int_0^\infty e^{-2r/a_0}\left(r^2-\frac{r^3}{a_0}\right)dr = \frac{4}{a_0^3}\left[2\left(\frac{a_0}{2}\right)^3 - \frac{6}{a_0}\left(\frac{a_0}{2}\right)^4\right] = -\frac{1}{2}. \end{aligned}$$

Thus, the probability is $1/4 = 0.25$.

(b) For $u_i = \psi_{100}(Z=1)$ and $v_j = \psi_{210}(Z=2)$ the θ-integral is

$$\int_0^\pi \cos\theta\sin\theta d\theta = \frac{1}{2}\int_0^\pi \sin 2\theta d\theta = \left[-\frac{\cos 2\theta}{4}\right]_0^\pi = 0.$$

For $u_i = \psi_{100}(Z=1)$ and $v_j = \psi_{21\pm1}(Z=2)$ the φ-integral is

$$\int_0^{2\pi} e^{\pm i\varphi}d\varphi = 0.$$

Thus, the probability to find the electron in a 2p state is zero.

(c) Here $u_i = \psi_{100}(Z=1)$ and $v_j = \psi_{100}(Z=2)$. This gives

$$\begin{aligned} a &= \left(\frac{1}{\pi a_0^3}\right)^{1/2}\left(\frac{2^3}{\pi a_0^3}\right)^{1/2}\int_0^\infty e^{-r/a_0}e^{-2r/a_0}4\pi r^2 dr = \frac{8\sqrt{2}}{a_0^3}\int_0^\infty e^{-3r/a_0}r^2 dr \\ &= \frac{8\sqrt{2}}{a_0^3}\frac{a_0^3}{3^3}\int_0^\infty e^{-x}x^2 dx = \frac{8\sqrt{2}}{27}\int_0^\infty e^{-x}x^2dx = \frac{8\sqrt{2}}{27}\int_0^\infty 2e^{-x}dx = \frac{16\sqrt{2}}{27} \end{aligned}$$

Thus, the probability is $512/729 \approx 0.70233$.
(The probability to find the electron in $\psi_{100}(Z=2)$ is $512/729 = 0.702$. Therefore, the electron is found with 95% probability in one of the states 1s or 2s.)

(d) No l has to be less than n.