LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS F0047T

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1. This is a 2 dimensional problem with a Schrödinger equation (where $V(x,y)=0$) like

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x,y)-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}\Psi(x,y)=E\Psi(x,y)$$

This equation is separable and the ansatz $\Psi(x,y)=\psi(x)*\psi(y)$ gives the following result

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_x(x)-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}\psi_y(y)=E_x\psi_x(x)+E_y\psi_y(y)$$

ie two independent one dimensional Schrödinger equations one for the variable x and on for y. We therefor solve the one dimensional problem first and after that we construct the two dimensional solution. To find the eigenfunctions we need to solve the Schrödinger equation which is (in the region where $V(x)$ is zero)

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi=E\Psi \;\rightarrow\; \frac{d^2}{dx^2}\Psi+k^2\Psi=0 \text{ where } k^2=\frac{2mE}{\hbar^2}$$

Solutions are of the kind:

$$\Psi(x)=A\cos kx+B\sin kx$$

Now we need to take the boundary conditions for the wave function Ψ $\left(\Psi(-\frac{a}{2})=\Psi(\frac{a}{2})=0\right)$ into account.

$$A\cos(-\frac{ka}{2})+B\sin(-\frac{ka}{2})=0 \text{ and } A\cos(\frac{ka}{2})+B\sin(\frac{ka}{2})=0$$

Adding the two conditions gives: $\cos(\frac{ka}{2})=0$ and subtracting them gives $\sin(\frac{ka}{2})=0$. These two conditions cannot be fulfilled at the same time, so either A or B has to be zero. We start with $A=0$ and we get the following solution: The normalising constant $B=\sqrt{\frac{2}{a}}$ you get from the condition $\int_{-a/2}^{a/2}\mid\Psi\mid^2 dx=1$. The condition $\sin(\frac{ka}{2})=0$ gives $\frac{ka}{2}=\frac{\pi}{2}*(even-integer)$. The solution is:

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a}) \text{ with eigenenergys } E_n=\frac{n^2\pi^2\hbar^2}{2Ma^2} \quad\text{where}\quad n=2,4,6,... \tag{1}$$

In a similar way the other function is analysed ($A=0$) which gives: The condition $\cos(\frac{ka}{2})=0$ gives $\frac{ka}{2}=\frac{\pi}{2}*(odd-integer)$. The solution is:

$$\psi_n(x)=\sqrt{\frac{2}{a}}\cos(\frac{n\pi x}{a}) \text{ with eigenenergys } E_n=\frac{n^2\pi^2\hbar^2}{2Ma^2} \quad\text{where}\quad n=1,3,5,... \tag{2}$$

The eigenfunctions in the y direction are the same as for the x direction as the potential is similar for this direction. Now we have the eigenfunctions of the one dimensional problem and the solution to the 2 dimensional problem is readily produced. The eigenfunctions are:

$$\Psi_{n,m}(x,y)=\psi_n(x)\cdot\psi_m(y) \text{ eigenenergys } E_{n,m}=E_n+E_m \text{where } n=1,2,,. \text{ and } m=1,2,,. \tag{3}$$

In the area where the potential is infinite the wave function is equal to zero.

An **alternative route** taken by many students has been to present a calculation with the following boundary conditions: Ψ ($\Psi(0) = \Psi(a) = 0$) into account. In this case the solution is for these boundary conditions:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a}) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1, 2, 3, ... \tag{4}$$

This solution has to be adapted to the boundary conditions related to this exam problem:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi}{a}(x+\frac{a}{2})) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1, 2, 3, ... \tag{5}$$

$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a} + \frac{n\pi}{2}) = \sqrt{\frac{2}{a}}\left(\sin(\frac{n\pi x}{a})\cdot\cos(\frac{n\pi}{2}) + \cos(\frac{n\pi x}{a})\cdot\sin(\frac{n\pi}{2})\right)$. We see that we recover the solution in eq (1), (2) and (3) as we let n run from 1 to ∞.

b) Now we turn to the question of **parity**, ie whether the wave function is *odd* or *even* under a change of coordinates from (x, y) to $(-x, -y)$. The one dimensional eigenfunctions in eq (1) and (2) have a definite parity. The functions in (1) are odd whereas the functions in (2) are even. As the eigenstates for the 2 dimensional system are formed from eq (3) ie products of functions that are even or odd the total function itself will be either even or odd as well.

The four lowest eigenenergies are given by

$$E_{n,m} = \frac{\pi^2\hbar^2}{2Ma^2}(n^2+m^2), \quad \text{where the 4 lowest are} \quad (n^2+m^2) = 2, 5, 8, 10.$$

When we form the eigenstates we need to keep track of the parity of the $\psi_n(x)$ and $\psi_m(y)$. It is therefore necessary to have the functions in the form like in eq (1) and (2) to identify the parity as odd or even. This is difficult if you try with functions like eq (5) even though it is a correct eigenstate it is hard to identify their parity.

$$\begin{aligned}
E_{1,1} =& \text{ one state } (n^2+m^2=2) && \text{even * even = even}\\
E_{1,2} = E_{2,1} =& \text{ two states } (n^2+m^2=5) && \text{even * odd = odd}\\
E_{2,2} =& \text{ one state } (n^2+m^2=8) && \text{odd * odd = even}\\
E_{1,3} = E_{3,1} =& \text{ two states } (n^2+m^2=10) && \text{even * even = even}
\end{aligned}$$

So of the four states only one is odd and three where even.

2. A measurement of the spin component in the direction $\hat{n} = \cos\varphi\hat{x} + \sin\varphi\hat{y}$ gives the value $\hbar/2$. The spin operator $S_{\hat{n}}$ is

$$S_{\hat{n}} = \frac{\hbar}{2}\begin{pmatrix} 0 & \cos\varphi - i\sin\varphi \\ \cos\varphi - i\sin\varphi & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{pmatrix}$$

The eigenvalue equation is

$$S_{\hat{n}}\chi = \lambda\chi \Leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix} \tag{6}$$

We find the eigenvalues from

$$\begin{vmatrix} -\lambda & \frac{\hbar}{2}e^{-i\varphi} \\ \frac{\hbar}{2}e^{i\varphi} & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm\frac{\hbar}{2}$$

(a) The spin state corresponding to $\lambda = +\hbar/2$ must satisfy the eigenvalue equation Eq. (6), *i.e.*

$$\chi_{\hat{n}+} = \begin{pmatrix} a \\ b \end{pmatrix} = b\begin{pmatrix} e^{-i\varphi} \\ 1 \end{pmatrix} \Rightarrow \chi_{\hat{n}+} = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\varphi} \\ 1 \end{pmatrix},$$

where the normalization condition $|a|^2 + |b|^2 = 1$ was used in the last step. Other correct solutions can be found by a multiplication with an arbitrary phase factor $\exp(i\alpha)$.

(b) A general spin state can be written as $\chi = a\chi_+ + b\chi_-$, where χ_+ is spin up and χ_- is spin down in z-direction. For $\chi_{\hat{n}+}$ we find that the probability to measure spin up, *i.e.* $S_z = \hbar/2$ is $|a|^2 = |e^{-i\varphi}/\sqrt{2}|^2 = 1/2$, and that the probability to measure spin down, *i.e.* $S_z = -\hbar/2$ is $|b|^2 = |1/\sqrt{2}|^2 = 1/2$.

3. (a) $\langle H\rangle = \frac{1}{2}0.31 + \frac{2}{12}0.97 + \frac{1}{12}1.81 + \frac{3}{16}3.35 + \frac{1}{16}4.08 = 1.350625 \approx 1.35\text{eV}$.
Uncertainty is defined by: $\langle \Delta H\rangle = \sqrt{\langle H^2\rangle - \langle H\rangle^2}$
$\langle H^2\rangle = \frac{1}{2}(0.31)^2 + \frac{2}{12}(0.97)^2 + \frac{1}{12}(1.81)^2 + \frac{3}{16}(3.35)^2 + \frac{1}{16}(4.08)^2 = 3.622494 \approx 3.62\text{eV}$.
$\langle \Delta H\rangle = \sqrt{3.622494 - 1.350625^2} = 1.341009 \approx 1.34\text{eV}$

(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: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \sqrt{\frac{2}{12}}\psi_2(z) + \frac{1}{\sqrt{12}}\psi_3(z) + \frac{\sqrt{3}}{4}\psi_4(z) + \frac{1}{4}\psi_5(z)$.
Another is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) - \sqrt{\frac{2}{12}}\psi_2(z) + \frac{1}{\sqrt{12}}\psi_3(z) + \frac{\sqrt{3}}{4}\psi_4(z) + \frac{1}{4}\psi_5(z)$.

(c) By a factor of 4. (All eigenvalues change by a factor of 4)

4. The task is to show that $\psi = Ae^{ax^2+bx}$ is the ground state. Rewrite the Schrödinger equation to

$$\frac{\partial^2}{\partial x^2}\psi = \frac{2m}{\hbar^2}\left(V(x) - E\right)\psi = \left[\frac{mk}{\hbar^2}x^2 - \frac{2mk}{\hbar^2}x_0 x + \frac{mk}{\hbar^2}x_0^2 - \frac{2mE}{\hbar^2}\right]Ae^{ax^2+bx} \tag{7}$$

$$\tag{8}$$

And form the derivatives of the function ψ:

$$\frac{\partial}{\partial x}\psi = (2ax+b)Ae^{ax^2+bx}; \tag{9}$$

$$\frac{\partial^2}{\partial x^2}\psi = (4a^2x^2 + 4abx + b^2 + 2a)Ae^{ax^2+bx} \tag{10}$$

$$\tag{11}$$

This yields $4a^2 = \frac{mk}{\hbar^2}$; $a = -\frac{\sqrt{mk}}{2\hbar}$, a must be less then 0 otherwise the wave function cannot be normalized.
Further $-\frac{2mk}{\hbar^2}x_0 = 4ab$ which gives $b = \frac{\sqrt{mk}}{\hbar}x_0$. Further $\frac{mk}{\hbar^2}x_0^2 - \frac{2mE}{\hbar^2} = b^2 + 2a = \frac{mk}{\hbar^2}x_0^2 - \frac{\sqrt{mk}}{\hbar}$ and this gives the energy $E = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$, ie the energy of the ground state. The constants are $a = -\frac{\sqrt{mk}}{2\hbar}$ and $b = \frac{\sqrt{mk}}{\hbar}x_0$.

5. 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

$$\psi(\boldsymbol{r}) = \psi(x, y, z) = N(zx)e^{-r/3a_0} = N\frac{r^2}{2}\sqrt{\frac{8\pi}{15}}(-Y_{2,1} + Y_{2,-1})e^{-r/3a_0} \ . \qquad (12)$$

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 know that n cannot be equal to 1 or 2 it has to be **larger** or **equal** to 3. By inspection of eq (12) 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 normailzed 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:

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

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