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) In Cartesian coordinates $r^2 = x^2 + y^2 + z^2$ and the Hamiltonian will be

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + \frac{m\omega^2}{2}\left(x^2 + y^2 + z^2\right).$$

$$H = -\frac{1}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{m\omega^2}{2}\left(x^2 + y^2 + z^2\right).$$

The Schroedinger (time independent) equation is

$$H\psi(x,y,z) = E\psi(x,y,z) \tag{1}$$

Make the ansatz for the wave function $\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z))$ . The Schroedinger equation (1) now is

$$\left(-\frac{1}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{m\omega^2}{2}\left(x^2 + y^2 + z^2\right)\right)\psi_x(x)\psi_y(y)\psi_z(z)) = E\psi_x(x)\psi_y(y)\psi_z(z))$$

This equation can be separated in the following way:

$$\left(-\frac{1}{2m}\left(\frac{1}{\psi_x(x)}\frac{\partial^2}{\partial x^2}\psi_x(x) + \frac{1}{\psi_y(y)}\frac{\partial^2}{\partial y^2}\psi_y(y) + \frac{1}{\psi_z(z)}\frac{\partial^2}{\partial z^2}\psi_z(z)\right) + \frac{m\omega^2}{2}\left(x^2 + y^2 + z^2\right)\right) = E$$

This equation splits into three independent functions one depends only on $x$ and one on $y$ and one on $z$. Let the constant $E = E_x + E_y + E_z$ and the three dimensional SE splits inte three one dimensional oscillators (below the one for $x$):

$$\left(-\frac{1}{2m}\left(\frac{1}{\psi_x(x)}\frac{\partial^2}{\partial x^2}\psi_x(x)\right) + \frac{m\omega^2}{2}\left(x^2\right)\right) = E_x$$

Where $E_x = \hbar\omega(n_x + \frac{1}{2})$ and the same for $E_y$ and $E_z$. The total energy is $E = \hbar\omega(n_x + n_y + n_z + \frac{3}{2})$. $n_x, n_y, n_z$ are independent integers =0, 1, 2, 3, ... .

b) From the collection of formulas we find for the one dimensional oscillator $\psi_{x0}(x) = \left(\frac{m\omega}{\hbar\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}m\omega x^2/\hbar}$. We can now formulate the ground state $n_x = n_y = n_z = 0$ for the 3 dimensional oscillator:

$$\psi_{000}(x,y,z) = \left(\frac{m\omega}{\hbar\sqrt{\pi}}\right)^{3/2} e^{-\frac{1}{2}m\omega x^2/\hbar} \cdot e^{-\frac{1}{2}m\omega y^2/\hbar} \cdot e^{-\frac{1}{2}m\omega z^2/\hbar}$$

c) Now we turn to the question of degeneration $d(n)$. As the energy is given by

$$E = \hbar\omega(n_x + n_y + n_z + \frac{3}{2})$$

we can assign $n = n_x + n_y + n_z$ to calculate the energy and $d(n)$ to count the number of states with the same energy, ie the number of combinations of $n_x, n_y, n_z$ that will result in the same energy.

We may try some combinations to get a feeling of how it works:

| $n$ | $d(n)$ | $n_x n_y n_z$ |
|---|---|---|
| 0 | 1 | 000 |
| 1 | 3 | $100, 010, 001$ |
| 2 | 6 | $\mathbf{200}, \mathbf{020}, 002,\ \mathbf{110}, 101, 011$ |
| 3 | 10 | $300, 030, 003,\ 111,\ 210, 201, 021, 120, 012, 102$ |

In the case of $n = 2$ the combinations with $n_z = 0$ have been marked with bold face These three points form a line in the $n_x, n_y$ plane this line contains 3 points (n+1). If we take the case of $n = 3$ the combinations with $n_z = 0$ will also form a line in the $n_x, n_y$ plane, this line containes 4 points (n+1). etc

Now wo consider the next layer with $n_z = 1$. In the case of $n = 2$ the combinations with $n_z = 1$ there are 2 points. In the case of $n = 3$ the combinations with $n_z = 1$ there are 3 points.

Now wo consider the next layer with $n_z = 2$. In the case of $n = 2$ the combinations with $n_z = 2$ there is 1 point. In the case of $n = 3$ the combinations with $n_z = 2$ there are 2 points.

Now wo consider the next layer with $n_z = 3$. In the case of $n = 2$ the combination with $n_z = 3$ not possible. In the case of $n = 3$ the combinations with $n_z = 3$ there is 1 point.

We see there is some order to these numbers as they form a triangle with n+1 points along each side. We can express this as follows starting from the base with n+1 we reach the top consisiting of only one point, this takes n+1 steps. There are n+1 rows and the average number of points in each row is ((n+1) +1)/2. Hence we can express the degeneration $d(n)$ as the product of the number of rows times the average number points on each row:

$$d(n) = (n+1)\frac{(n+2)}{2}$$

2. 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 $\Psi$ $\left(\Psi(-\frac{a}{2}) = \Psi(\frac{a}{2}) = 0\right)$ 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:

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

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:

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

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:

$$\Psi_{n,m}(x, y) = \psi_n(x) \cdot \psi_m(y) \text{ eigenenergys } E_{n,m} = E_n + E_m \text{where } n = 1, 2, , . \text{ and } m = 1, 2, , . \tag{4}$$

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: $\Psi$ $(\Psi(0) = \Psi(a) = 0)$ into account. In this case the solution is for these boundary conditions:

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

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

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi}{a}(x + \frac{a}{2})) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1, 2, 3, ... \tag{6}$$

$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a} + \frac{n\pi}{2}) = \sqrt{\frac{2}{a}}\left(\sin(\frac{n\pi x}{a}) \cdot \cos(\frac{n\pi}{2}) + \cos(\frac{n\pi x}{a}) \cdot \sin(\frac{n\pi}{2})\right)$. We see that we recover the solution in eq (2), (3) and (4) as we let $n$ run from 1 to $\infty$.

**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 (2) and (3) have a definite parity. The functions in (2) are odd whereas the functions in (3) are even. As the eigenstates for the 2 dimensional system are formed from eq (4) 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

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

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 (2) and (3) to identify the parity as odd or even. This is difficult if you try with functions like eq (6) even though it is a correct eigenstate it is hard to identify their parity.

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

So of the four energys (states) only one is **odd** and three are **even**.

3. **Spin**

Suppose a spin 1/2 particle is in the state

$$\chi = \frac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ 1+i \end{pmatrix}.$$

(a) What are the probabilities of getting $+\hbar/2$ and $-\hbar/2$ , if you mesure $S_{\mathbf{z}}$?

(b) What are the probabilities of getting $+\hbar/2$ and $-\hbar/2$ , if you mesure $S_{\mathbf{y}}$?

(3p)

The appropriate spin opperators are

$$S_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } S_z = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

a) For $S_z$ the eigenvalues are $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ and the eigenspinors are for the positive eigenvalue $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and for the negative eigenvalue $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. We have to express the given spinor in terms of the eigenspinors to $S_z$ in the following expansion:

$$\chi = \frac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \frac{1+i}{\sqrt{6}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \frac{2}{\sqrt{6}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1+i}{\sqrt{6}}\chi_- + \frac{2}{\sqrt{6}}\chi_+$$

The probabillities are now just the absolute squares of the coefficients in the expansion above.

The probabillity to get $-\frac{\hbar}{2}$ is $\frac{2}{6} = \frac{1}{3}$

The probabillity to get $+\frac{\hbar}{2}$ is $\frac{4}{6} = \frac{2}{3}$

b) For $S_y$ we have to do some calculations to find the appropriate eigenspinors. The eigenvalue equation is

$$S_y\chi = \lambda\chi \;\Leftrightarrow\; \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix} \tag{7}$$

We find the eigenvalues from

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

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

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

This gives two identical equations $-ib = a$. Now let $a = 1$ and hence $b = i$. This gives the unnormalised spinor

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

For the negative eigenvalue we get the $-a = -ib$ and hence the eigen spinor is

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

Now we have to express the given spinor in terms of the eigenspinors to $S_y$:

$$\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ 1+i \end{pmatrix}$$

We make use of the projection by operating from the left with $\chi^*_{y+}$:

$$\chi^*_{y+}\chi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \end{pmatrix} * \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \frac{2 + -i(1+i)}{\sqrt{12}} = \frac{3-i}{\sqrt{12}}$$

For the other spinor we find (operating from the left with $\chi^*_{y-}$):

$$\chi^*_{y-}\chi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \end{pmatrix} * \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \frac{2 + i(1+i)}{\sqrt{12}} = \frac{1+i}{\sqrt{12}}$$

Now we know howto expand $\chi$ in the eigenspinors of $S_y$

$$\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \frac{3-i}{\sqrt{12}}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} + \frac{1+i}{\sqrt{12}}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{3-i}{\sqrt{12}}\cdot\chi_{y+} + \frac{1+i}{\sqrt{12}}\cdot\chi_{y-}$$

The probabillities are now just the absolute squares of the coefficients in the expansion above.

The probabillity to get $+\frac{\hbar}{2}$ is $\frac{10}{12} = \frac{5}{6}$

The probabillity to get $-\frac{\hbar}{2}$ is $\frac{2}{12} = \frac{1}{6}$

4. (a) i. $\hat{\Pi}C\left(\cos(\frac{\pi x}{L})+\cos(\frac{3\pi x}{L})\right)=C\left(\cos(\frac{-\pi x}{L})+\cos(\frac{-3\pi x}{L})\right)=+C\left(\cos(\frac{\pi x}{L})+\cos(\frac{3\pi x}{L})\right)$ , the eigenvalue is $+1$

ii. $\hat{\Pi}Ce^{-a\sqrt{x^2+3y^2+z^2}}=Ce^{-a\sqrt{(-x)^2+3(-y)^2+(-z)^2}}=Ce^{-a\sqrt{x^2+3y^2+z^2}}$ , the eigenvalue is $+1$

iii. $\hat{\Pi}Cf(r)\left(\cos(\theta)+cos^3(\theta)\right)\ e^{i\phi}=Cf(r)\left(\cos(\pi-\theta)+cos^3(\pi-\theta)\right)\ e^{i(\phi+\pi)}=Cf(r)\left(-\cos(\theta)+-cos^3(\theta)\right)\ (-e^{i\phi})=Cf(r)\left(\cos(\theta)+cos^3(\theta)\right)\ e^{i\phi}$ , the eigenvalue is $+1$

(b) i. $\hat{\Pi}(4\psi_+(x,y,z)+2\psi_-(x,y,z))=+4\psi_+(x,y,z)+-2\psi_-(x,y,z)\neq\lambda(4\psi_+(x,y,z)+2\psi_-(x,y,z))$ , not an eigenfunction.

ii. $\hat{\Pi}^2(4\psi_+(x,y,z)+2\psi_-(x,y,z))=\hat{\Pi}(+4\psi_+(x,y,z)+-2\psi_-(x,y,z))=4\psi_+(x,y,z)+2\psi_-(x,y,z)$ , an eigenfunction with eigenvalue $+1$.

iii. $\hat{\Pi}e^{-\alpha x}=e^{+\alpha x}\neq e^{-\alpha x}$ not an eigenfunction and neither is $e^{+\alpha x}$. We can however form linear combinations that have parity. The function $e^{\alpha x}-e^{-\alpha x}$ has parity $\hat{\Pi}e^{+\alpha x}-e^{-\alpha x}=e^{-\alpha x}-e^{+\alpha x}=-1(e^{+\alpha x}-e^{-\alpha x})$ with eigenvalue -1. The function $e^{+\alpha x}+e^{-\alpha x}$ has parity $\hat{\Pi}e^{+\alpha x}+e^{-\alpha x}=e^{-\alpha x}+e^{+\alpha x}=+1(e^{+\alpha x}+e^{-\alpha x})$ with eigenvalue $+1$.

5. (a) The total wave function has to be normalised which implies that the sum of the squared coefficients equals one. $A^2(2^2+3^2+1^1+1^2)=1$ resulting in $A^2=\frac{1}{15}$ and hence $A=\frac{1}{\sqrt{15}}$.

(b) The probability is given by the absolute square of the coefficients.
$(\Psi(\mathbf{r},t=0)=\frac{1}{\sqrt{15}}\left(2\psi_{100}(\mathbf{r})-3\psi_{211}(\mathbf{r})+\psi_{320}(\mathbf{r})-\psi_{322}(\mathbf{r})\right))$

The probabilities are (in order) $\frac{4}{15}$, $\frac{9}{15}$, $\frac{1}{15}$, $\frac{1}{15}$. as a check they sum up to 1 as they should do.

(c) The energy of a single eigenstate is given by: $E_n=-\frac{13.56}{n^2}$ eV. The expectation value is given by $<E>=\frac{4}{15}(-\frac{13.56}{1^2})+\frac{9}{15}(-\frac{13.56}{2^2})+\frac{1}{15}(-\frac{13.56}{3^2})+\frac{1}{15}(-\frac{13.56}{3^2})=-13.56(\frac{4}{15}+\frac{9}{60}+\frac{1}{135}+\frac{1}{135})=-13.56\frac{233}{540}=-5.807868\approx-5.81$ eV

The operator $\mathbf{L}^2$ has eigenvalues $\hbar^2l(l+1)$. The expectation value is given by $<\mathbf{L^2}>=\frac{4}{15}\cdot0+\frac{9}{15}\cdot(\hbar^2 1(1+1))+\frac{1}{15}(\hbar^2 2(2+1))+\frac{1}{15}(\hbar^2 2(2+1))=\frac{30}{15}\hbar^2=2\hbar^2$

The operator $L_z$ has eigenvalues $\hbar m_l$. The expectation value is given by $<L_z>=\frac{4}{15}\cdot0+\frac{9}{15}\cdot1\hbar+\frac{1}{15}\cdot0+\frac{1}{15}(2\hbar)=\frac{11}{15}\hbar$