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. 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.

$E_{1,1} =$ one state $(n^2 + m^2 = 2)$ **even * even** = even

$E_{1,2} = E_{2,1} =$ two states $(n^2 + m^2 = 5)$ odd * even = odd

$E_{2,2} =$ one state $(n^2 + m^2 = 8)$ **odd * odd** = even

$E_{1,3} = E_{3,1} =$ two states $(n^2 + m^2 = 10)$ **even * even** = even

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

2. (a) Let the commutator act on a wave function $\Psi(x)$ and $p_x = -i\hbar\frac{d}{dx}$
$[x^2, p_x^2]\Psi(x) = -\hbar^2(x^2\frac{d^2\Psi(x)}{dx^2} - \frac{d^2(x^2\Psi(x))}{dx^2}) = -\hbar^2\left(x^2\frac{d^2\Psi(x)}{dx^2} - x^2\frac{d^2\Psi(x)}{dx^2} - 4x\frac{d\Psi(x)}{dx} - 2\Psi(x)\right) =$
$+\hbar^2 2\Psi(x) + 4x\hbar^2\frac{d\Psi(x)}{dx} = \left(+\hbar^2 2 + i4\hbar x p_x\right)\Psi(x)$ concluding for the commutator:
$[x^2, p_x^2] = +2\hbar^2 + 4i\hbar x p_x$.

   (b) The energy levels for a hydrogen like system are given by: $E_n = -13.6\frac{Z^2}{n^2}$ [eV], here we have $Z = +3$: $\Delta E = E(2s) - E(1s) = E_2 - E_1 = -13.54 \cdot (\frac{9}{2^2} - \frac{9}{1^2}) = 13.54 \cdot \frac{27}{4} = 91,53$ eV

(c) The angular part of the wave function can be written as a spherical harmonic:

$$3\cos^2\theta - 1 \propto Y_{20}$$

Which gives $l = 2$ och $m = 0$. The part depending on r $(r^2/a_\mu^2)e^{-r/3a_\mu}$ corresponding to the principal quantum number $n = 3$ och $l = 2$ consistent with Y_{20}.

3. Rewrite $L_z^2 + L_y^2 = L^2 - L_x^2$, which gives the Hamiltonian

$$H = \frac{L^2 - L_x^2}{2\hbar^2} + \frac{L_x^4}{4\hbar^2} = \frac{L^2 - L_x^2}{4\hbar^2}.$$

Here we use the freedom to orient the coordinate system such that the appropriate operators are L_x and L^2 instead of the usual conventional L_z and L^2. The eigenfunctions are not the ordinary spherical harmonics but we know the eigenvalue spectrum that is the same. Lets denote the eigenfunctions by $\tilde{Y}_{l,m_x}$

$$H\tilde{Y}_{l,m_x} = \left(\frac{L^2 - L_x^2}{2\hbar^2} + \frac{L_x^2}{4\hbar^2}\right)\tilde{Y}_{l,m_x} = \left(\frac{l(l+1)\hbar^2 - m_x^2\hbar^2}{2\hbar^2} + \frac{m_x^2\hbar^2}{4\hbar^2}\right)\tilde{Y}_{l,m_x}.$$

Hence the energies are:

$$E_{l,m_x} = \left(\frac{l(l+1)}{2} - \frac{m_x^2}{4}\right).$$

An important issue is the relation between l and m_x, ie $l = 0, 1, 2, 3, ...$ and $m_x = -l, -l+1, ..., 0, l-1, l$. Or it may also be expressed through some kind of treatment where it from the treatment is clear how l and m_x are related. The lowest (ground state) energy is $E_{0,0} = 0$ ($l = 0$ no rotation).

$l = 1 \rightarrow m_x = 0, \pm 1$, gives $E_{1,0} = \frac{2}{2} = 1\text{eV}$ $E_{1,\pm1} = \frac{3}{4}\text{eV}$

$l = 2 \rightarrow m_x = 0, \pm 1, \pm 2$, gives $E_{2,0} = 3\text{eV}$ $E_{2,\pm1} = \frac{11}{4}\text{eV}$ $E_{2,\pm2} = 2\text{eV}$

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5. (a) There are several ways to determine A. One is to integrate and use the normalization condition to solve for A. A different path (done here) is to write the given wave function in terms of eigenfunctions. The eigenfunctions are (PH) $\psi(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$. We can directly conclude that the given wave function consists of eigenfunctions with $n = 1$ and $n = 5$, we can write:

$$\psi(x,0) = \frac{A\sqrt{2}}{\sqrt{2a}}\sin\left(\frac{\pi x}{a}\right) + \frac{\sqrt{2}}{\sqrt{2\cdot 5a}}\sin\left(\frac{5\pi x}{a}\right) = \frac{A}{\sqrt{2}}\psi_1(x,0) + \frac{1}{\sqrt{10}}\psi_5(x,0)$$

As both eigenfunctions are orthonormal the normalisation integral reduces to $\frac{A^2}{2} + \frac{1}{10} = 1$ and hence $A = \sqrt{\frac{18}{10}} = \sqrt{\frac{9}{5}} = \frac{3}{\sqrt{5}}$

(b) The wave function contains only $n = 1$ and $n = 5$ eigenfunctions and therefore the only possible outcomes of an energy meassurement are $E_1 = \frac{\hbar^2\pi^2}{2ma^2}$ with probability $\frac{A^2}{2} = 0.9$ and $E_5 = \frac{\hbar^2\pi^2}{2ma^2}25$ with probability 1 - 0.9 = 0.1 . The average energy is given by $< E >= 0.9E_1 + 0.1E_5 = \frac{\hbar^2\pi^2}{2ma^2}(0.9 + 0.1\cdot 25) = 3.4\cdot\frac{\hbar^2\pi^2}{2ma^2} = 1.7\cdot\frac{\hbar^2\pi^2}{ma^2}$

(c) The time dependent solution is given by $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$ and hence

$$\Psi(x,t) = \sqrt{\frac{9}{10}}\psi_1(x,0)e^{-i\frac{\hbar\pi^2 t}{2ma^2}} + \frac{1}{\sqrt{10}}\psi_5(x,0)e^{-i\frac{25\hbar\pi^2 t}{2ma^2}}$$

6. (a) The mean position of the particle is

$$< x >= \int_{-\infty}^{\infty} \psi^*(x) x \psi^*(x) dx = \frac{\gamma}{\sqrt{\pi}} \int_{-\infty}^{\infty} x e^{-\gamma^2 x^2} dx = 0$$

(b) The mean momentum of the particle is

$$< p >= \int_{-\infty}^{\infty} \psi^*(x) \frac{\hbar}{i} (\frac{d}{dx}\psi(x)) dx = \frac{\gamma\hbar}{\sqrt{i\pi}} \int_{-\infty}^{\infty} e^{-\gamma^2 x^2/2} \frac{d}{dx} e^{-\gamma^2 x^2/2} dx = 0$$

(c) The Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x)$$

can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = [E - V(x)]\psi(x).$$

As

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} e^{-\gamma^2 x^2/2} = -\frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2) e^{-\gamma^2 x^2/2}$$

we have

$$E - V(x) = -\frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2)$$

or

$$V(x) = \frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2) + \frac{\hbar^2\gamma^2}{2m} = \frac{\hbar^2\gamma^4 x^2}{2m}$$