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) 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 (here particle in a box). The eigenfunctions are (PH) $\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$. We can directly conclude that the given wave function consists of $n = 1$, $n = 5$ and $n = 7$ functions, we can write:

$$\psi(x,0) = \frac{\sqrt{13\cdot 2}}{\sqrt{8\cdot 2\cdot a}}\sin\left(\frac{\pi x}{a}\right) + \frac{\sqrt{2}}{2\sqrt{2\cdot a}}\sin\left(\frac{5\pi x}{a}\right) + \frac{A\sqrt{2}}{\sqrt{2\cdot a}}\sin\left(\frac{7\pi x}{a}\right) =$$

$$\frac{\sqrt{13}}{\sqrt{16}}\psi_1(x,0) + \frac{1}{\sqrt{8}}\psi_5(x,0) + \frac{A}{\sqrt{2}}\psi_7(x,0)$$

As all three eigenfunctions are orthonormal the normalisation integral reduces to $\frac{13}{16} + \frac{1}{8} + \frac{A^2}{2} = 1$ and hence $A = \frac{1}{2\sqrt{2}} = \frac{\sqrt{2}}{4} = \frac{1}{\sqrt{8}} = (\approx 0.3536)$.

(b) The wave function contains only $n = 1$, $n = 5$ and $n = 7$ eigenfunctions and therefore the only possible outcomes of an energy meassurement are $E_1 = \frac{\hbar^2\pi^2}{2ma^2}$ with probability $\frac{13}{16}$ and $E_5 = \frac{\hbar^2\pi^2}{2ma^2}25$ with probability $\frac{1}{8}$ and $E_7 = \frac{\hbar^2\pi^2}{2ma^2}49$ with probability $\frac{A^2}{2} = \frac{1}{16}$.
The average energy is given by
$< E >= \frac{13}{16}E_1 + \frac{1}{8}E_5 + \frac{1}{16}E_7 = \frac{\hbar^2\pi^2}{2ma^2}(\frac{13}{16} + \frac{1}{8}\cdot 25 + \frac{1}{16}\cdot 49) = \frac{112}{16}\cdot\frac{\hbar^2\pi^2}{2ma^2} = 7\cdot\frac{\hbar^2\pi^2}{2ma^2}$

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

$$\Psi(x,t) = \sqrt{\frac{13}{16}}\psi_1(x,0)e^{-i\frac{\hbar\pi^2 t}{2ma^2}} + \frac{1}{\sqrt{8}}\psi_5(x,0)e^{-i\frac{25\hbar\pi^2 t}{2ma^2}} + \frac{1}{4}\psi_7(x,0)e^{-i\frac{49\hbar\pi^2 t}{2ma^2}}$$

2. Same/similar as problem 4.4 in Bransden & Joachain. In the region where the potential is zero ($x < 0$) the solutions are of the traveling wave form e^{ikx} and e^{-ikx}, where $k^2 = 2mE/\hbar^2$. A plane wave $\psi(x) = Ae^{i(kx-\omega t)}$ describes a particle moving from $x = -\infty$ towards $x = \infty$. The probability current associated with this plane wave is
$j = \frac{\hbar}{2mi} \mid A\mid^2 (e^{-ikx}\frac{\partial}{\partial x}e^{+ikx} - e^{+ikx}\frac{\partial}{\partial x}e^{-ikx}) =\mid A\mid^2 \frac{\hbar}{m}k =\mid A\mid^2 v$
A plane wave $\psi(x) = Be^{i(-kx-\omega t)}$ describes a particle moving the opposite direction from $x = \infty$ towards $x = -\infty$. The probability current associated with this plane wave is
$j = \frac{\hbar}{2mi} \mid B\mid^2 (e^{+ikx}\frac{\partial}{\partial x}e^{-ikx} - e^{-ikx}\frac{\partial}{\partial x}e^{+ikx}) = -\mid B\mid^2 \frac{\hbar}{m}k = -\mid B\mid^2 v$

a Solution for the region $x > 0$ where the potential is $V_0 = 4.5$eV. The potential step is larger than the kinetic energy 2.0 eV of the incident beam. The particle may therefore **not** enter this region classically. It will be totally reflected. In quantum mechanics we perform the following calculation: The two solutions for the two regions are:

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for} \quad x < 0 \quad \text{where} \quad k^2 = 2mE/\hbar^2 \\ Ce^{\kappa x} + De^{-\kappa x} & \text{for} \quad x > 0 \quad \text{where} \quad \kappa^2 = 2m(V_0 - E)/\hbar^2 \end{cases}$$

we can put $C = 0$ as this part of the solution would diverge, and is hence not physical, as x approaches ∞. At $x = 0$ both the wavefunction and its derivative have to be continous functions, as the potential is everywhere finite. The derivative is:

$$\frac{\partial\Psi(x)}{\partial x} = \begin{cases} Aike^{ikx} - Bike^{-ikx} \\ -D\kappa e^{-\kappa x} \end{cases}$$

At $x = 0$ we arrive at the following two equations:

$$\begin{cases} A + B = D \\ iAk - iBk = -D\kappa \end{cases} \text{solving for} \begin{cases} \frac{D}{A} = \frac{2k}{k+\kappa} \\ \frac{B}{A} = \frac{k-i\kappa}{k+i\kappa} \end{cases} \text{solving for} \begin{cases} \frac{D}{A} = \frac{2}{1+i\sqrt{V_0/E-1}} \\ \frac{B}{A} = \frac{1-i\sqrt{V_0/E-1}}{1+i\sqrt{V_0/E-1}} \end{cases}$$

We can now calculate the coeficient of reflection, R The coeficients represent the following amplitudes: A is the incident beam, B is the reflected beam and C is the transmitted beam. The associated probability currents are denoted j_A, j_B and j_C. Conservation yields $j_A = j_B + j_C$. Hence we can define the coeficient of reflection as the fraction of reflected flux $R = \frac{|j_B|}{|j_A|}$ and the coeficient of transmission as $T = \frac{|j_C|}{|j_A|}$

$$\begin{cases} R = \frac{|j_B|}{|j_A|} = \frac{B^2k}{A^2k} = 1 \end{cases}$$

This is easily seen from the ratio B/A being the ratio of two complex number where one is the complex conjugate of the other and therefore having the same absolute value. Imidiately follows that $T = 0$ as the currents have to be conserved.

(b+c) Solution for the region $x > 0$ where the potential is $V_0 = 4.5$eV. The potential step is smaller than the kinetic energy 7.0eV or 5.0eV of the incident beam. The particle may therefore enter this region classically. It will however lose some of its kinetic energy. In quantum mechanics there is a probabillity for the wave to be reflected as well. The two solutions for the two regions are:

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for} \quad x < 0 \quad \text{where} \quad k^2 = 2mE/\hbar^2 \\ Ce^{ik'x} + De^{-ik'x} & \text{for} \quad x > 0 \quad \text{where} \quad k'^2 = 2m(E - V_0)/\hbar^2 \end{cases}$$

whe can put $D = 0$ as there cannot be an incident beam from $x = \infty$. At $x = 0$ both the wavefunction and its derivative have to be continous functions. The derivative is:

$$\frac{\partial\Psi(x)}{\partial x} = \begin{cases} Aike^{ikx} - Bike^{-ikx} \\ Cik'e^{ik'x} \end{cases}$$

At $x = 0$ we arrive at the following two equations:

$$\begin{cases} A + B = C \\ Ak - Bk = Ck' \end{cases} \text{solving for} \begin{cases} \frac{C}{A} = \frac{2k}{k+k'} \\ \frac{B}{A} = \frac{k-k'}{k+k'} \end{cases} \text{solving for} \begin{cases} \frac{C}{A} = \frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}} \\ \frac{B}{A} = \frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}} \end{cases}$$

The coeficients represent the following amplitudes: A is the incident beam, B is the reflected beam and C is the transmitted beam. The associated probability currents are denoted j_A, j_B and j_C. Conservation yields $j_A = j_B + j_C$. Hence we can define the coeficient of reflection as the fraction of reflected flux $R = \frac{|j_B|}{|j_A|}$ and the coeficient of transmission as $T = \frac{|j_C|}{|j_A|}$ For the two cases in part b and c the coeficients are:

$$\begin{cases} R = \frac{|j_B|}{|j_A|} = \frac{B^2k}{A^2k} = \left(\frac{B}{A}\right)^2 = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 = \left(\frac{\sqrt{5.0}-\sqrt{0.5}}{\sqrt{5.0}+\sqrt{0.5}}\right)^2 = 0.26987 \\ T = \frac{|j_C|}{|j_A|} = \frac{C^2k'}{A^2k} = \left(\frac{C}{A}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{5.0}}{\sqrt{5.0}+\sqrt{0.5}}\right)^2 \frac{\sqrt{0.5}}{\sqrt{5.0}} = 0.73013 \end{cases}$$

$$\begin{cases} R = \frac{|j_B|}{|j_A|} = \frac{B^2 k}{A^2 k} = \left(\frac{B}{A}\right)^2 = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 = \left(\frac{\sqrt{7.0}-\sqrt{2.5}}{\sqrt{7.0}+\sqrt{2.5}}\right)^2 = 0.063437 \\ T = \frac{|j_C|}{|j_A|} = \frac{C^2 k'}{A^2 k} = \left(\frac{C}{A}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{7.0}}{\sqrt{7.0}+\sqrt{2.5}}\right)^2 \frac{\sqrt{2.5}}{\sqrt{7.0}} = 0.936563 \end{cases}$$

The last result could also be reached by $T + R = 1$.

3. The harmonic oscillator eigenfunction of the ground state is

$$\psi_0(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}}\, e^{-\frac{1}{2}\alpha^2 x^2} \text{ where } \alpha = \sqrt{\frac{m\omega}{\hbar}}.$$

The four expectation values we are asked to calculate are $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, $\langle p^2\rangle$ by explicit integration. By arguments of symmetry we find that $\langle x\rangle = 0$ and the same is for $\langle p\rangle = 0$, as both will be integrals of an odd function that approaches zero exponentially as the arguments go to $\pm\infty$.

The first integral to calculate (use integration by parts) will be for $\langle x^2\rangle$

$$\langle 0 \mid x^2 \mid 0\rangle = \int \psi_0^*(x) x^2 \psi_0(x) dx = \int \frac{\alpha}{\sqrt{\pi}} x^2\ e^{-\alpha^2 x^2} dx = [\alpha x = y] = \frac{1}{\alpha^2\sqrt{\pi}} \int y^2\ e^{-y^2} dy$$

where the integral taken separatelly will be

$$\int_{-\infty}^{\infty} y^2\ e^{-y^2} dy = [-\frac{y^1}{2} e^{-y^2}]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{1}{2} e^{-y^2} = 0 + \frac{1}{2}\sqrt{\pi} = \frac{\sqrt{\pi}}{2}$$

and we arrive at:

$$\langle 0 \mid x^2 \mid 0\rangle = \frac{1}{\alpha^2\sqrt{\pi}} \frac{\sqrt{\pi}}{2} = \frac{1}{2\alpha^2} \quad (= \frac{\hbar}{2m\omega})$$

Note on dimensions. As an argument of an exponential function has to be dimensionless this requires the product αx to be dimensionless. As x has dimension 'length' the dimension of α has to be '1/length'. So the expression for $\langle x^2\rangle$ has to contain a one over α squared in order to have the correct dimension.

For the second integral $\langle p^2\rangle$ we have ($p = -i\hbar\frac{\partial}{\partial x}$)

$$\langle 0 \mid p^2 \mid 0\rangle = \int \psi_0^*(x) p^2 \psi_0(x) dx = \int \frac{\alpha}{\sqrt{\pi}} e^{-\frac{1}{2}\alpha^2 x^2} (-i\hbar\frac{\partial}{\partial x})^2\ e^{-\frac{1}{2}\alpha^2 x^2} dx =$$

$$-\hbar^2 \int \frac{\alpha}{\sqrt{\pi}} e^{-\frac{1}{2}\alpha^2 x^2} \alpha^2(\alpha^2 x^2 - 1) e^{-\frac{1}{2}\alpha^2 x^2} dx = -\hbar^2 \langle 0 \mid (\alpha^2(\alpha^2 x^2 - 1) \mid 0\rangle =$$

$$-\hbar^2 \left(\alpha^2 \langle 0 \mid \alpha^2 x^2 \mid 0\rangle - \langle 0 \mid \alpha^2 \mid 0\rangle\right) = -\hbar^2 \left(\alpha^4 \frac{1}{2\alpha^2} - \alpha^2\right) = \frac{1}{2}\hbar^2\alpha^2 \quad (= \frac{1}{2}\hbar m\omega)$$

Uncertainty is defined by: $\langle \Delta p\rangle = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$ and as both $\langle x\rangle$ and $\langle p\rangle$ are zero we arrive at:

$$\langle \Delta p\rangle\langle \Delta x\rangle = \sqrt{\frac{1}{2}\hbar^2\alpha^2 \cdot \frac{1}{2\alpha^2}} = \hbar\frac{1}{2} = \frac{\hbar}{2}$$

which is larger or equal to $\frac{\hbar}{2}$ as it should be according to the uncertainty principal.

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

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

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

i+ii together give 0.5 (both correct) and iii gives 1.0 p

(b) i. $\hat{\Pi}(2\psi_+(x,y,z)+3\psi_-(x,y,z)) = +2\psi_+(x,y,z)+-3\psi_-(x,y,z) \neq \lambda(2\psi_+(x,y,z)+3\psi_-(x,y,z))$, not an eigenfunction.

ii. $\hat{\Pi}^2(2\psi_+(x,y,z)+3\psi_-(x,y,z)) = \hat{\Pi}(+2\psi_+(x,y,z)+-3\psi_-(x,y,z)) =$ $2\psi_+(x,y,z)+3\psi_-(x,y,z)$, an eigenfunction with eigenvalue +1.

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

i+ii together give 0.5 (both correct) and iii gives 1.0 p

5. 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:

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

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) The ground state eigenfunction is given by (using eq. (2))

$$\Psi_{n=1,m=1}(x, y) = \psi_1(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \cos(\frac{\pi x}{a}) \cdot \sqrt{\frac{2}{a}} \cos(\frac{\pi y}{a}) \tag{6}$$

The next lowest state eigenfunction is given by (using eq. (2) and (1)). Note there are two eigenfunctions with the same energy ($\Psi_{n=1,m=2}(x, y)$) you may use either one of them.

$$\Psi_{n=2,m=1}(x, y) = \psi_2(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \sin(2\frac{\pi x}{a}) \cdot \sqrt{\frac{2}{a}} \cos(\frac{\pi y}{a}) \tag{7}$$

Orthogonality is defined as

$$\int_x \int_y \Psi_{n_1,m_1}(x, y)\Psi_{n_2,m_2}(x, y) = \delta_{n_1,n_2} \; \delta_{m_1,m_2} \tag{8}$$

by explicit calculation

$$\int_{x=-a/2}^{a/2} \int_{y=-a/2}^{a/2} \left(\frac{2}{a} \cos(\frac{\pi x}{a}) \cdot \cos(\frac{\pi y}{a})\right) \cdot \left(\frac{2}{a} \sin(2\frac{\pi x}{a}) \cdot \cos(\frac{\pi y}{a})\right) = \text{calculations} = 0 \tag{9}$$

this is a separable integral (in x and y), suggestion do the integral in x first as this will be zero as they belong to different eigenvalues. Thus the calculation ends with a zero as it should.