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. 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 $T = \frac{|j_C|}{|j_A|}$

$$\left\{ R = \frac{|j_B|}{|j_A|} = \frac{B^2k}{A^2k} = 1 \right.$$

   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:

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

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

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

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 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) 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.

3. The eigenfunctions and eigenvalues of the free-particle Hamiltonian are found by solving the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V(x)u(x) = Eu(x),$$

with $V(x)$ zero everywhere. Thus, the eigenvalue equation reads

$$\frac{d^2u(x)}{dx^2} + k^2u(x) = 0,$$

where $k^2 = 2mE/\hbar^2$. The eigenfunctions are given by the plane waves e^{ikx} and e^{-ikx}, or linear combinations of these, as *e.g.* $\sin kx$ and $\cos kx$.

(a) The wave function of the particle at $t = 0$ is given by

$$\psi(x,0) = \cos^3(kx) + \sin^3(kx).$$

This is not an eigenfunction in itself but it can be written as sum of eigenfunctions using the Euler relations

$$\psi(x,0) = \left(\frac{e^{ikx}+e^{-ikx}}{2}\right)^3 + \left(\frac{e^{ikx}-e^{-ikx}}{2i}\right)^3 = \tag{10}$$

$$\frac{1}{8}\left(e^{i3kx}+3e^{ikx}+3e^{-ikx}+e^{-i3kx}\right) - \frac{1}{8i}\left(e^{i3kx}-3e^{ikx}+3e^{-ikx}-e^{-i3kx}\right) = \tag{11}$$

$$\frac{3}{4}\cos(kx) + \frac{1}{4}\cos(3kx) + \frac{3}{4}\sin(kx) - \frac{1}{4}\sin(3kx) \tag{12}$$

Thus, $\psi(x,0)$ can be written as a superposition of plane waves with two different values of $k_1 = k$ and $k_2 = 3k$.

(b) The energy of a plane wave e^{ikx} is given by $E = \hbar^2 k^2/2m$. Thus, the energy of $e^{ik_1 x}$ (or $e^{-ik_1 x}$) is $E_1 = \hbar^2 k^2/2m$ and the energy of $e^{ik_2 x}$ (or $e^{-ik_2 x}$) is $E_2 = \hbar^2 k_2^2/2m = 9\hbar^2 k^2/2m$.

(c) The function $u(x) = e^{ikx}$ is a solution to the the time-independent Schrödinger equation. The corresponding solutions to the time-dependent Schrödinger equation are given by $u(x)T(t)$,with $T(t) = e^{-iEt/\hbar}$. Therefore, $u(x)T(t) = e^{i(kx - Et/\hbar)}$. A sum of solutions of this form is also a solution, since the Schrödinger equation is linear. This means that if $\psi(x, 0)$ is given by equation (12), then the time dependent solution is given by

$$\psi(x,t) = \frac{1}{8}\left(e^{i3kx} + e^{-i3kx}\right)e^{-iE_2 t/\hbar} + \frac{3}{8}\left(e^{ikx} + e^{-ikx}\right)e^{-iE_1 t/\hbar} + \tag{13}$$

$$\frac{1}{8i}\left(e^{i3kx} - e^{-i3kx}\right)e^{-iE_2 t/\hbar} - \frac{3}{8i}\left(e^{ikx} - e^{-ikx}\right)e^{-iE_1 t/\hbar} \tag{14}$$

where

$$E_1 = \frac{\hbar^2 k^2}{2m} \quad \text{and} \quad E_2 = \frac{9\hbar^2 k^2}{2m} \tag{15}$$

4. A measurement of the spin in the direction $\hat{n} = \sin(\frac{\pi}{4})\hat{e}_y + \cos(\frac{\pi}{4})\hat{e}_z = \frac{1}{\sqrt{2}}\hat{e}_y + \frac{1}{\sqrt{2}}\hat{e}_z$. The spin operator $S_{\hat{n}}$ is

$$S_{\hat{n}} = \frac{1}{\sqrt{2}}S_y + \frac{1}{\sqrt{2}}S_z = \frac{\hbar}{2\sqrt{2}}\begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}$$

The eigenvalue equation is

$$S_{\hat{n}}\chi = \lambda\chi \Leftrightarrow \frac{\hbar}{2\sqrt{2}}\begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix} \tag{16}$$

We find the eigenvalues from

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

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

$$\frac{\hbar}{2\sqrt{2}}\begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = +\frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}$$

$$\frac{a}{\sqrt{2}} - \frac{ib}{\sqrt{2}} = a \Leftrightarrow a(\sqrt{2} - 1) = -ib \;\; \text{let} \;\; b = 1 \;\; \text{and hence} \;\; a = \frac{-i}{\sqrt{2} - 1}$$

This gives the unnormalised spinor

$$\begin{pmatrix} -\frac{i}{\sqrt{2}-1} \\ 1 \end{pmatrix} \quad \text{and after normalisation we have} \quad \chi_{\hat{n}+} = \frac{1}{\sqrt{2(2+\sqrt{2})}}\begin{pmatrix} -\frac{i}{\sqrt{2}-1} \\ 1 \end{pmatrix}$$

Now we can expand the initial eigenspinor χ_+ in these eigenspinors to S_n, the second eigenspinor you can get from orthogonality to the first one.

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = A\frac{1}{\sqrt{2(2+\sqrt{2})}}\begin{pmatrix} -\frac{i}{\sqrt{2}-1} \\ 1 \end{pmatrix} + B\frac{1}{\sqrt{2(2+\sqrt{2})}}\begin{pmatrix} 1 \\ \frac{-i}{\sqrt{2}-1} \end{pmatrix}$$

The coefficients are subjected to the normalisation condition $|A|^2 + |B|^2 = 1$. The coefficient A can be obtained by multiplying the previous equation from the left with $\chi^*_{\hat{n}+}$.

$$A = \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} -\frac{i}{\sqrt{2}-1} & 1 \end{pmatrix} * \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\frac{i}{\sqrt{2}-1} \cdot \frac{1}{\sqrt{2(2+\sqrt{2})}}$$

The probability (to get $+\frac{\hbar}{2}$) is given by $|A|^2$.

$$|A|^2 = \frac{3+2\sqrt{2}}{4+2\sqrt{2}} = 0.8535533906$$

and (to get $-\frac{\hbar}{2}$) for $|B|^2$.

$$|B|^2 = \frac{1}{4+2\sqrt{2}} = 0.1464466094$$

To find the probability for $+\frac{\hbar}{2}$ in the z-direction for the up state of S_n express the state in the eigenspinors to S_z.

$$\chi_{\hat{n}+} = \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} -\frac{i}{\sqrt{2}-1} \\ 1 \end{pmatrix} = -\frac{i}{\sqrt{2}-1} \cdot \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The probability is given by the square of the coefficient:

$$\left| -\frac{i}{\sqrt{2}-1} \cdot \frac{1}{\sqrt{2(2+\sqrt{2})}} \right|^2 = 0.8535533906$$

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

(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 $Z = 4 : \Delta E = E(2s) - E(1s) = E_2 - E_1 = -13.54 \cdot (\frac{16}{2^2} - \frac{16}{1^2}) = 13.54 \cdot \frac{16 \cdot 3}{4} = 162.48$ 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}.