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) Let the commutator act on a wave function $\Psi(y)$ and $p_y = -i\hbar\frac{d}{dy}$
$[y^2, p_y^2]\Psi(y) = -\hbar^2(y^2\frac{d^2\Psi(y)}{dy^2} - \frac{d^2(y^2\Psi(y))}{dy^2}) = -\hbar^2\left(y^2\frac{d^2\Psi(y)}{dy^2} - y^2\frac{d^2\Psi(y)}{dy^2} - 4y\frac{d\Psi(y)}{dy} - 2\Psi(y)\right) =$
$+\hbar^2 2\Psi(y) + 4y\hbar^2\frac{d\Psi(y)}{dy} = (+\hbar^2 2 + i4\hbar y p_y)\,\Psi(y)$ 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 $Y_{20}$.

2. (a) The parity of a hydrogen eigenfunction $\psi_{nlm_l}(\mathbf{r})$ is given by $(-1)^l$. The given wave function $\Psi(\mathbf{r})$ consists of eigenfunctions with different parity. Hence $\Psi(\mathbf{r})$ has no definite parity.

   (b) The probability is given by the absolute square of the coefficients.
$(\Psi(\mathbf{r}, t = 0) = \frac{1}{\sqrt{15}}\left(3\psi_{100}(\mathbf{r}) - 2\psi_{210}(\mathbf{r}) + \psi_{310}(\mathbf{r}) - \psi_{322}(\mathbf{r})\right))$
The probabilities are (in order) $\frac{9}{15}, \frac{4}{15}, \frac{1}{15}, \frac{1}{15}$. 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 $< E >= \frac{9}{15}(-\frac{13.56}{1^2}) + \frac{4}{15}(-\frac{13.56}{2^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) =$
$-13.56(\frac{9}{15} + \frac{4}{60} + \frac{1}{135} + \frac{1}{135}) = -9.240889 \approx -9.24$ eV
The operator $\mathbf{L}^2$ has eigenvalues $\hbar^2 l(l+1)$. The expectation value is given by
$< \mathbf{L^2} >= \frac{9}{15}\cdot 0 + \frac{4}{15}(\hbar^2 1(1+1)) + \frac{1}{15}(\hbar^2 1(1+1)) + \frac{1}{15}(\hbar^2 2(2+1)) = \frac{4\cdot 2+2+6}{15}\hbar^2 = \frac{16}{15}\hbar^2$
The operator $L_z$ has eigenvalues $\hbar m_l$. The expectation value is given by
$< L_z >= \frac{9}{15}\cdot 0 + \frac{4}{15}\cdot 0 + \frac{1}{15}\cdot 0 + \frac{1}{15}(\hbar 2) = \frac{2}{15}\hbar$

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

$$H = \frac{L^2 - L_z^2}{2\hbar^2} + \frac{L_z^2}{3\hbar^2}.$$

   The eigenfunctions are $Y_{l,m}$

$$HY_{l,m} = \left(\frac{L^2 - L_z^2}{2\hbar^2} + \frac{L_z^2}{3\hbar^2}\right)Y_{l,m} = \left(\frac{l(l+1)\hbar^2 - m^2\hbar^2}{2\hbar^2} + \frac{m^2\hbar^2}{3\hbar^2}\right)Y_{l,m}.$$

   Hence the energies are:

$$E_{l,m} = \left(\frac{l(l+1)}{2} - \frac{m^2}{6}\right).$$

The lowest (ground state) energy is $E_{0,0} = 0$ ($l = 0$ no rotation).
$l = 1 \rightarrow m = 0, \pm 1$, gives $E_{1,0} = 1\text{eV}$ $E_{1,\pm 1} = \frac{5}{6}\text{eV}$
$l = 2 \rightarrow m = 0, \pm 1, \pm 2$, gives $E_{2,0} = 3\text{eV}$ $E_{2,\pm 1} = \frac{17}{6}\text{eV}$ $E_{2,\pm 2} = \frac{7}{3}\text{eV}$
and so on.

4. a) There are 4 states the system can have with the energys and (degeneracys) $\hbar\omega$ (1), $2\hbar\omega$ (2) and $3\hbar\omega$ (1). The partition sum is given by:

$$Z = \sum_{n_1=0,n_2=0}^{n_1=1,n_2=1} e^{-(n_1+n_2+1.0)\hbar\omega/k_BT} = e^{-1.0\hbar\omega/k_BT} + 2e^{-2.0\hbar\omega/k_BT} + e^{-3.0\hbar\omega/k_BT}$$

b) There is one state of the lower energy and there are **two** states with the next higher energy. The probability to find the system in a state of energy is proportional to the Boltzmann factor, we arrive at the following equation for the probabilities.

$$\frac{1e^{-1,0\hbar\omega/k_BT}}{Z} = \frac{2e^{-2,0\hbar\omega/k_BT}}{Z} \tag{1}$$

and this reduces to $e^{1\hbar\omega/k_BT} = 2$ which evaluates to $T = \frac{1\hbar\omega}{k_B \ln 2}$ .

c) The partition sum at this specific temperature is given by: ($k_BT = \frac{1\hbar\omega}{\ln 2}$) ($\frac{1}{k_BT} = \frac{\ln 2}{1\hbar\omega}$) we arrive at the following

$$Z = e^{-1.0\hbar\omega/k_BT} + 2e^{-2.0\hbar\omega/k_BT} + e^{-3.0\hbar\omega/k_BT} = e^{-1.0\ln 2} + 2e^{-2.0\ln 2} + e^{-3.0\ln 2} =$$

$$\frac{1}{2} + 2\frac{1}{4} + \frac{1}{8} = \frac{1}{2} + \frac{1}{2} + \frac{1}{8} = 1 + \frac{1}{8} = \frac{9}{8}$$

The probability $P$ will be (put $Z$ into one of the terms in eq (1).

$$P = \frac{e^{-1,0\ln 2}}{\frac{9}{8}} = \frac{1}{2} \cdot \frac{8}{9} = \frac{4}{9} \approx 0.444...$$

*As a check we can calculate for the state with the highest energy*

$$P_3 = \frac{e^{-3,0\ln 2}}{\frac{9}{8}} = \frac{1}{8} \cdot \frac{8}{9} = \frac{1}{9} \approx 0.111...$$

*and we can easily conclude the probabilities add up to one.*

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

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

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:

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

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

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