LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

# Solution to written exam in QUANTUM PHYSICS F0047T

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1. Same 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 $V_0 = 3.5$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. 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 coefficient of reflection, $R$, the ratio between the reflected flux $j_B$ and the incoming flux $j_A$. 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 $V_0 = 3.5$eV. The potential step is smaller than the kinetic energy 5.0eV (or 7.0eV) 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 $T = \frac{|j_C|}{|j_A|}$

$$E = 5.0 \begin{cases} R = \frac{|j_B|}{|j_A|} = \frac{B^2 k}{A^2 k} = \left(\frac{B}{A}\right)^2 = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 = \left(\frac{\sqrt{5.0}-\sqrt{1.5}}{\sqrt{5.0}+\sqrt{1.5}}\right)^2 = 0.085393 \\ T = \frac{|j_C|}{|j_A|} = \frac{C^2 k'}{A^2 k} = \left(\frac{C}{A}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{5.0}}{\sqrt{5.0}+\sqrt{1.5}}\right)^2 \frac{\sqrt{1.5}}{\sqrt{5.0}} = 0.914607 \end{cases}$$

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

$$E = 7.0 \begin{cases} R = \frac{|j_B|}{|j_A|} = \frac{B^2 k}{A^2 k} = \left(\frac{B}{A}\right)^2 = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 = \left(\frac{\sqrt{7.0}-\sqrt{3.5}}{\sqrt{7.0}+\sqrt{3.5}}\right)^2 = 0.029437 \\ T = \frac{|j_C|}{|j_A|} = \frac{C^2 k'}{A^2 k} = \left(\frac{C}{A}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{7.0}}{\sqrt{7.0}+\sqrt{3.5}}\right)^2 \frac{\sqrt{3.5}}{\sqrt{7.0}} = 0.970563 \end{cases}$$

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

2. (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:

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

$$\frac{A}{2}\psi_1(x,0) + \frac{1}{\sqrt{8}}\psi_5(x,0) + \frac{1}{4}\psi_7(x,0)$$

As all three eigenfunctions are orthonormal the normalisation integral reduces to $\frac{A^2}{4} + \frac{1}{8} + \frac{1}{16} = 1$ and hence $A = \frac{\sqrt{13}}{2} (\approx 1.8028)$.

(b) The wave function contains only $n=1$, $n=5$ and $n=7$ eigenfunctions and therefore the only possible outcome of an energy meassurement are $E_1 = \frac{\hbar^2\pi^2}{2ma^2}$ with probability $\frac{A^2}{4} = \frac{13}{16}$ 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 $\frac{1}{16}$.
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

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

3. (a) $i\hbar\frac{\partial^2}{\partial t^2}\sin\omega t = i\hbar\omega\frac{\partial}{\partial t}\cos\omega t = -i\hbar\omega^2\sin\omega t$ **YES**

(b) $-i\hbar\frac{\partial}{\partial z}C(1+z^2) = -i\hbar C(0+2z)$ **NO**

(c) $-i\hbar\frac{\partial^2}{\partial z^2}(C_1e^{ikz} + C_2e^{-ikz}) = -i\hbar ik\frac{\partial}{\partial z}(C_1e^{ikz} - C_2e^{-ikz}) = -i\hbar k^2(C_1e^{ikz} + C_2e^{-ikz})$ **YES**

(d) $-\frac{\hbar}{2}\frac{\partial}{\partial z}Ce^{-3z} = -\frac{\hbar}{2}C(-3)e^{-3z} \propto \psi(z)$ **YES**

(e) $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} =?$ This has to be done in some steps. Start by doing this derivative first: $-\frac{\partial^2}{\partial z^2}ze^{-\frac{1}{2}z^2} = -\frac{\partial}{\partial z}(e^{-\frac{1}{2}z^2} - z^2e^{-\frac{1}{2}z^2}) = -(-ze^{-\frac{1}{2}z^2} - 2ze^{-\frac{1}{2}z^2} + z^3e^{-\frac{1}{2}z^2}) = 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}$.
Now you go back to the start: $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} = \frac{C}{2}(z^3e^{-\frac{1}{2}z^2} + 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}) = \frac{C}{2}(+3ze^{-\frac{1}{2}z^2}) = \propto \psi(z)$ **YES**

(f) $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})e^{-\frac{1}{2}z^2} = \frac{C}{2}(z^2e^{-\frac{1}{2}z^2} - \frac{\partial}{\partial z}(-ze^{-\frac{1}{2}z^2})) = \frac{C}{2}(z^2e^{-\frac{1}{2}z^2} - (-e^{-\frac{1}{2}z^2} + z^2e^{-\frac{1}{2}z^2})) = \frac{C}{2}e^{-\frac{1}{2}z^2} \propto \psi(z)$ **YES**

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

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

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

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

Now we can expand the initial eigenspinor $\chi_+$ 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. Molekylens energinivåer, pga vibrationer och rotation ges av $E_{n,l} = (n+\frac{1}{2})\hbar\omega + \frac{\hbar^2}{2I}l(l+1)$ Vid dipolövergång ändras $l$ med en enhet $\Delta l = \pm 1$.

   **I)** Om vibrationstillståndet **ej** ändras ($\Delta n = 0$), ser man strålning med följande energier $\frac{\hbar^2}{2I}(l+1)(l+2) - \frac{\hbar^2}{2I}l(l+1) = \frac{\hbar^2}{I}(l+1), l = 0,1,2,3,$ och detta ger $\frac{\hbar^2}{I}, 2\frac{\hbar^2}{I}, 3\frac{\hbar^2}{I}, 4\frac{\hbar^2}{I}, ...$
   **II)** Om vibrationstillståndet ändras **en** enhet $\Delta n = -1$ (emission), ser man två serier, där avståndet mellan energinivåerna för varje serie är lika stort. Ena serien har $\Delta n = -1, \Delta l = -1$: $\hbar\omega + \frac{\hbar^2}{I}, \hbar\omega + 2\frac{\hbar^2}{I}, \hbar\omega + 3\frac{\hbar^2}{I}, \hbar\omega + 4\frac{\hbar^2}{I}, ...$ Den andra serien har $\Delta n = -1, \Delta l = +1$: $\hbar\omega - \frac{\hbar^2}{I}, \hbar\omega - 2\frac{\hbar^2}{I}, \hbar\omega - 3\frac{\hbar^2}{I}, \hbar\omega - 4\frac{\hbar^2}{I}, ...$

   Det ser alltså ut som om det 'saknas' en topp med energin $\hbar\omega$.

   Avståndet mellan maxima svarar mot $\Delta E = \frac{\hbar^2}{I} = hc\Delta\lambda^{-1}$ ur data fås $\Delta\lambda^{-1} = \frac{2968.7-2824.0}{7} = 20.67\text{cm}^{-1}$ vidare är $I = \mu R^2 = \frac{m_H m_{Cl}}{m_H + m_{Cl}}$ och därmed $R = \sqrt{\frac{h}{4\pi^2 c\Delta\lambda^{-1}\mu}} = 1.30\text{Å}$.