LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Quantum Physics F0047T

Examination date: 2010-08-18

1. The eigenfunctions of the infinite square well are (Physics handbook)

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \quad \text{and the eigenenergies are } E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad \text{where} \quad n = 1, 2, 3, ...$$

The correction to the eigenenergies due to perturbation is given by:

$$E_n^1 =< H_1 > \quad \text{where} \quad H_1 \text{ is the deviation in the potential from the infinite square well.}$$

$$E_n^1 = \int_0^{a/2} \frac{2\epsilon}{a} \sin^2 \frac{n\pi x}{a} dx = \int_0^{a/2} \frac{2\epsilon}{a2} \left(1 - \cos \frac{2n\pi x}{a}\right) dx = \frac{\epsilon}{a} \left[x - \frac{a}{2n\pi} \sin \frac{2n\pi x}{a}\right]_0^{a/2} = \frac{\epsilon}{2}$$

This is the same for all n. The corrections for n=1 and n=2 are of intrest (**answer to a)**).

$$E_1^1 = E_2^1 = \frac{\epsilon}{2} = 0.315\text{eV}.$$

The two lowest eigenergies are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{n^2h^2}{8ma^2} \quad [n=1] \quad E_1 = 3.76540625 \cdot 10^{-19}\text{J} = 2.350175\text{eV} \quad \text{and} \quad E_2 = 9.4007125\text{eV}$$

To calculate the transition energy between two perturbed levels we first calculate the new energys, due to the perturbation, for the two lowest levels:

$$E_1^* = 2.350175 + 0.315 = 2.665175\text{eV} \quad \text{and} \quad E_2^* = 9.4007125 + 0.315 = 9.71571251.559114\text{eV}$$

The transition energy between the perturbed levels will be 9.7157125 - 2.665175 = 7.0505375 eV. The same would be for the unperturbed levels as the perturbation changes all levels by the same energy (to first order).

2. 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 $V_0 = 5.0$eV. The potential step is larger than the kinetic energy 2.5 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. 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 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) This case can be seen as either the limiting case of a) or c). Both give the same answer $R = 1$ and $T = 0$.

(c) Solution for the region $x > 0$ where the potential is $V_0 = 5.0$eV. The potential step is smaller than the kinetic energy 7.5eV 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 $T = \frac{|j_C|}{|j_A|}$

$$\begin{cases} R = \frac{|j_B|}{|j_A|} = \frac{B^2 k}{A^2 k} = \left(\frac{B}{A}\right)^2 = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 = \left(\frac{\sqrt{7.5}-\sqrt{2.5}}{\sqrt{7.5}+\sqrt{2.5}}\right)^2 = 0.071797 \\ T = \frac{|j_C|}{|j_A|} = \frac{C^2 k'}{A^2 k} = \left(\frac{C}{A}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{7.5}}{\sqrt{7.5}+\sqrt{2.5}}\right)^2 \frac{\sqrt{2.5}}{\sqrt{7.5}} = 0.928203 \end{cases}$$

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

3. Hydrogenic atoms have eigenfunctions $\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta, \varphi)$. Using the COLLECTION OF FORMULAE we find

$$\begin{aligned} \psi_{100}(\boldsymbol{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0} \\ \psi_{200}(\boldsymbol{r}) &= \left(\frac{Z^3}{8\pi a_0^3}\right)^{1/2} \left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0} \\ \psi_{210}(\boldsymbol{r}) &= \left(\frac{Z^3}{32\pi a_0^3}\right)^{1/2} \frac{Zr}{a_0} \cos\theta e^{-Zr/2a_0} \\ \psi_{21\pm1}(\boldsymbol{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} \frac{Zr}{8a_0} \sin\theta e^{\pm i\varphi} e^{-Zr/2a_0} \end{aligned}$$

where a_0 is the Bohr radius. The β-decay instantaneously changes $Z = 1 \to Z = 2$. According to the expansion theorem, it is possible to express the wave function $u_i(\boldsymbol{r})$ before the decay as a linear combination of eigenfunctions $v_j(\boldsymbol{r})$ after the decay as

$$u_i(\boldsymbol{r}) = \sum_j a_j v_j(\boldsymbol{r})$$

where

$$a_j = \int v_j^*(\boldsymbol{r}) u_i(\boldsymbol{r}) d^3 r.$$

The probability to find the electron in state j is given by $|a_j|^2$.

(a) Here $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{200}(Z = 2)$. This gives

$$\begin{aligned} a &= \left(\frac{1}{\pi a_0^3}\right)^{1/2} \left(\frac{2^3}{8\pi a_0^3}\right)^{1/2} \int_0^\infty e^{-r/a_0} \left(1 - \frac{2r}{2a_0}\right) e^{-2r/2a_0} 4\pi r^2 dr \\ &= \frac{4}{a_0^3} \int_0^\infty e^{-2r/a_0} \left(r^2 - \frac{r^3}{a_0}\right) dr = \frac{4}{a_0^3} \left[2\left(\frac{a_0}{2}\right)^3 - \frac{6}{a_0}\left(\frac{a_0}{2}\right)^4\right] = -\frac{1}{2}. \end{aligned}$$

Thus, the probability is $1/4 = 0.25$.

(b) For $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{210}(Z = 2)$ the θ-integral is

$$\int_0^\pi \cos\theta \sin\theta d\theta = \frac{1}{2} \int_0^\pi \sin 2\theta d\theta = \left[-\frac{\cos 2\theta}{4}\right]_0^\pi = 0.$$

For $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{21\pm1}(Z = 2)$ the φ-integral is

$$\int_0^{2\pi} e^{\pm i\varphi} d\varphi = 0.$$

Thus, the probability to find the electron in a 2p state is zero.

(c) Here $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{100}(Z = 2)$. This gives

$$\begin{aligned} a &= \left(\frac{1}{\pi a_0^3}\right)^{1/2} \left(\frac{2^3}{\pi a_0^3}\right)^{1/2} \int_0^\infty e^{-r/a_0} e^{-2r/a_0} 4\pi r^2 dr = \frac{8\sqrt{2}}{a_0^3} \int_0^\infty e^{-3r/a_0} r^2 dr \\ &= \frac{8\sqrt{2}}{a_0^3} \frac{a_0^3}{3^3} \int_0^\infty e^{-x} x^2 dx = \frac{8\sqrt{2}}{27} \int_0^\infty e^{-x} x^2 dx = \frac{8\sqrt{2}}{27} \int_0^\infty 2e^{-x} dx = \frac{16\sqrt{2}}{27} \end{aligned}$$

Thus, the probability is $512/729 \approx 0.70233$.

(The probability to find the electron in $\psi_{100}(Z = 2)$ is $512/729 = 0.702$. Therefore, the electron is found with 95% probability in one of the states 1s or 2s.)

(d) No l has to be less than n.

4. (a) To show that $\psi^+(\xi) = A\xi e^{+\xi^2/2}$ solves the differential equation put it in! The first derivative and second derivatives are (A cancels out):

$$\frac{d\psi^+(\xi)}{d\xi} = e^{+\xi^2/2} + \xi^2 e^{+\xi^2/2} \quad \text{and} \quad \frac{d^2\psi^+(\xi)}{d\xi^2} = \xi e^{+\xi^2/2} + 2\xi e^{+\xi^2/2} + \xi^3 e^{+\xi^2/2} = 3\xi e^{+\xi^2/2} + \xi^3 e^{+\xi^2/2}$$

Now evaluate the following:

$$\frac{d^2\psi^+(\xi)}{d\xi^2} + (\lambda^+ - \ \xi^2)\psi^+(\xi) = (\lambda^+ + 3)\xi e^{+\xi^2/2} + \xi^3 e^{+\xi^2/2} - \xi^3 e^{+\xi^2/2} = (\lambda^+ + 3)\xi e^{+\xi^2/2} = 0$$

If $\lambda^+ = -3$ the desired result is reached.

The same yields for $\psi^-(\xi) = B\xi e^{-\xi^2/2}$. The first derivative and second derivatives are (B cancels out):

$$\frac{d\psi^-(\xi)}{d\xi} = e^{-\xi^2/2} - \xi^2 e^{-\xi^2/2} \quad \text{and} \quad \frac{d^2\psi^-(\xi)}{d\xi^2} = -\xi e^{-\xi^2/2} - 2\xi e^{-\xi^2/2} + \xi^3 e^{-\xi^2/2} = -3\xi e^{-\xi^2/2} + \xi^3 e^{-\xi^2/2}$$

Now evaluate the following:

$$\frac{d^2\psi^-(\xi)}{d\xi^2} + (\lambda^- - \ \xi^2)\psi^-(\xi) = (\lambda^- - 3)\xi e^{-\xi^2/2} + \xi^3 e^{-\xi^2/2} - \xi^3 e^{-\xi^2/2} = (\lambda^- - 3)\xi e^{-\xi^2/2} = 0$$

If $\lambda^- = +3$ the desired result is reached.

(b) Only one is physical acceptable $\psi^-(\xi)$ as it can be normalised. The othe function $\psi^+(\xi)$ is not acceptable as it cannot be normalized and therefore it does not describe a particle.

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 $n = 1$ and $n = 5$ functions, 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 outcome 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

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