LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Quantum Physics F0047T

Examination date: 2017-08-26
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 $V_0 = 4.5\text{eV}$. 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 $T + R = 1$.

2. 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 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:

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

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

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

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

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

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 $E = \hbar^2k^2/2m$. Thus, the energy of e^{ik_1x} (or e^{-ik_1x}) is $E_1 = \hbar^2k^2/2m$ and the energy of e^{ik_2x} (or e^{-ik_2x}) is $E_2 = \hbar^2k_2^2/2m = 9\hbar^2k^2/2m$.

(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 (4), then the time dependent solution is given by

$$\psi(x,t) = \frac{1}{8}\left(e^{i3kx}+e^{-i3kx}\right)e^{-iE_2t/\hbar} + \frac{3}{8}\left(e^{ikx}+e^{-ikx}\right)e^{-iE_1t/\hbar} + \quad (5)$$

$$\frac{1}{8i}\left(e^{i3kx}-e^{-i3kx}\right)e^{-iE_2t/\hbar} - \frac{3}{8i}\left(e^{ikx}-e^{-ikx}\right)e^{-iE_1t/\hbar} \quad (6)$$

where

$$E_1 = \frac{\hbar^2k^2}{2m} \quad \text{and} \quad E_2 = \frac{9\hbar^2k^2}{2m} \quad (7)$$

4. The task is to calculate the change of the energy levels (ground state E_0 and first excited state E_1) for a harmonic oscillator due to a perturbation H^1 to the potential.

The two harmonic oscillator eigenfunctions that are of interest are :

$$\psi_0(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}}\, e^{-\frac{1}{2}\alpha^2x^2} \quad \text{and} \quad \psi_1(x) = \sqrt{\frac{\alpha}{2\sqrt{\pi}}}2\alpha x\, e^{-\frac{1}{2}\alpha^2x^2} \quad \text{where} \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}$$

(a) Here we have a perturbation γx^4 where γ is small in some sence. The first integral to calculate (use integration by parts) will be for the change of the ground state energy

$$\langle 0 \mid \gamma x^4 \mid 0\rangle = \int \psi_0^*(x)\gamma x^4\psi_0(x)dx = \int \frac{\alpha}{\sqrt{\pi}}\gamma x^4\, e^{-\alpha^2x^2}dx = [\alpha x = y] = \frac{\gamma}{\alpha^4\sqrt{\pi}}\int y^4\, e^{-y^2}dy$$

where the integral taken separately will be

$$\int_{-\infty}^{\infty} y^4\, e^{-y^2}dy = [-\frac{y^3}{2}e^{-y^2}]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\frac{3y^2}{2}e^{-y^2} = [-\frac{3y^1}{4}e^{-y^2}]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\frac{3}{4}e^{-y^2} = \frac{3}{4}\sqrt{\pi}$$

Hence the shift of the ground state energy will be

$$\langle 0 \mid \gamma x^4 \mid 0\rangle = \frac{\gamma}{\alpha^4\sqrt{\pi}}\frac{3}{4}\sqrt{\pi} = \frac{3\gamma}{4\alpha^4} = \frac{3\gamma}{4}\left(\frac{\hbar}{m\omega}\right)^2$$

The energy of the unperturbed groundstate is $E_0 = \frac{\hbar\omega}{2}$. Hence the energy of the perturbed groundstate is

$$E_0^{\text{perturbed}} = \frac{\hbar\omega}{2} + \frac{3\gamma}{4}\left(\frac{\hbar}{m\omega}\right)^2$$

(b) Here we have a perturbation ϵx where ϵ is small in some sence. The integrals to be calculated are $\langle 0 \mid \epsilon x \mid 0\rangle$ and $\langle 1 \mid \epsilon x \mid 1\rangle$. The squares of both eigenfunctions are even functions and as the perturbation is odd both integrals will be zero.

Hence there is no change in energy to first order.

5. (a) As

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos(\theta) \quad \text{and} \quad Y_{1,\pm 1} = \sqrt{\frac{3}{8\pi}}\sin(\theta)e^{\pm\phi}$$

the wave function can be written as

$$\psi = \frac{1}{4\pi}\left(e^{i\phi}\sin(\theta) + \cos(\theta)\right)g(r) = \sqrt{\frac{1}{3}}(-\sqrt{2}Y_{1,1} + Y_{1,0})g(r).$$

Hence the possible values of L_z are $+\hbar$ and 0.

(b) Since

$$\int \mid \psi \mid^2 = \frac{1}{4\pi}\int_0^\infty \mid g(r) \mid^2 r^2 dr \int_0^\pi d\theta \int_0^{2\pi}(1+\cos\phi\sin 2\theta)\sin\theta d\phi = \frac{1}{2}\int_0^\pi \sin\theta \; d\theta = 1,$$

the given wave function is normalised. The probability density is then given by $P = \mid \psi \mid^2$. Thus the probability of $L_z = +\hbar$ is $\mid \sqrt{\frac{2}{3}} \mid^2 = \frac{2}{3}$ and that of $L_z = 0$ is $\mid \sqrt{\frac{1}{3}} \mid^2 = \frac{1}{3}$.

(c) The expectation value of L_z is

$$< L_z > = \mid \sqrt{\frac{2}{3}} \mid^2 (+\hbar) + \mid \sqrt{\frac{1}{3}} \mid^2 (0) = \frac{2}{3}\hbar$$