LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS AND STATISTICAL PHYSICS F0018T / MTF131

Examination date: 2008-12-19
Note solutions are more detailed compared to previous solutions, earlier than October 2007.

1. Same as problem 4.4 in Bransden & Joachain. In the region where the potential is zero ($x < 0$) the solutions are of the travelling 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 $V_0 = 10.0$eV. The potential step is larger than the kinetic energy 5eV 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:

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for} \quad x < 0 \quad \text{where} \quad k^2 = 2mE/\hbar^2 \\ Ce^{\kappa x} + De^{-\kappa x} & \text{for} \quad x > 0 \quad \text{where} \quad \kappa^2 = 2m(V_0 - E)/\hbar^2 \end{cases}$$

   whe 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 coefficients 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 yealds $j_A = j_B + j_C$. Hence we can define the coefficient of reflection as the fraction of reflected flux $R = \frac{|j_B|}{|j_A|}$ and the coefficient 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. Immediately follows that $T = 0$ as the currents have to be conserved.

(b) Solution for the region $x > 0$ where the potential is $V_0 = 10.0$eV. The potential step is smaller than the kinetic energy 15eV 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 probability for the wave to be reflected as well. The two solutions for the two regions are:

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for} \quad x < 0 \quad \text{where} \quad k^2 = 2mE/\hbar^2 \\ Ce^{ik'x} + De^{-ik'x} & \text{for} \quad x > 0 \quad \text{where} \quad k'^2 = 2m(E - V_0)/\hbar^2 \end{cases}$$

we can put $D = 0$ as there cannot be an incident beam from $x = \infty$. At $x = 0$ both the wave function and its derivative have to be continuous 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 coefficients 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 yealds $j_A = j_B + j_C$. Hence we can define the coefficient of reflection as the fraction of reflected flux $R = \frac{|j_B|}{|j_A|}$ and the coefficient of transmission as $T = \frac{|j_C|}{|j_A|}$

$$\begin{cases} R = \frac{|j_B|}{|j_A|} = \frac{B^2k}{A^2k} = \left(\frac{B}{A}\right)^2 = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 = \left(\frac{\sqrt{15}-\sqrt{5}}{\sqrt{15}+\sqrt{5}}\right)^2 = 0.07180 \\ T = \frac{|j_C|}{|j_A|} = \frac{C^2k'}{A^2k} = \left(\frac{C}{A}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{15}}{\sqrt{15}+\sqrt{5}}\right)^2 \frac{\sqrt{5}}{\sqrt{15}} = 0.9282 \end{cases}$$

(c) This case can be seen as either the limiting case of a) or b). Both give the same answer $R = 1$ and $T = 0$.

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

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

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. (a) $\langle H \rangle = \frac{1}{2}0.31 + \frac{2}{12}0.97 + \frac{1}{12}1.81 + \frac{3}{16}3.35 + \frac{1}{16}4.08 = 1.350625 \approx 1.35\text{eV}$.

   Uncertainty is defined by: $\langle \Delta H \rangle = \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$

   $\langle H^2 \rangle = \langle H \rangle = \frac{1}{2}(0.31)^2 + \frac{2}{12}(0.97)^2 + \frac{1}{12}(1.81)^2 + \frac{3}{16}(3.35)^2 + \frac{1}{16}(4.08)^2 = 3.622494 \approx 3.62\text{eV}$.

   $\langle \Delta H \rangle = \sqrt{3.622494 - 1.350625^2} = 1.341009 \approx 1.34\text{eV}$

   (b) The expression is not unique as we only know the probabilities which are the squares of the coefficients. In the evaluation of $\langle H \rangle$ and $\langle H^2 \rangle$ only the probabilities are important thats why a different sign $\pm$ is of no importance in this calculation.

   One is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \sqrt{\frac{2}{12}}\psi_2(z) + \frac{1}{\sqrt{12}}\psi_3(z) + \frac{\sqrt{3}}{4}\psi_4(z) + \frac{1}{4}\psi_5(z)$.

   Another is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) - \sqrt{\frac{2}{12}}\psi_2(z) + \frac{1}{\sqrt{12}}\psi_3(z) + \frac{\sqrt{3}}{4}\psi_4(z) + \frac{1}{4}\psi_5(z)$.

(c) By a factor of 4. (All eigenvalues change by a factor of 4)

4. The line that is special (due to intensity) is $\lambda = 470.22$nm with intensity 200. The Helium ion has $Z = 2$ and hence energys $E_n = -\frac{54.24}{n^2}$eV. Try to find a start of the series. The energy of $\lambda = 658.30$nm is $E = h\nu = \frac{hc}{\lambda} = \frac{6.626 \cdot 10^{-34} \cdot 2.9979 \cdot 10^8}{6.5830 \cdot 10^{-7} \cdot 1.6022 \cdot 10^{-19}} = 1.8833$eV A similar calculation gives for the other lines in the series: 2.28306, 2.54250, 2.72037, 2.84760, 2.94174, 3.01333, 3.06905 and for the special line 2.63667eV

   As Balmer series in Hydrogen is for transitions down to level n=2 we have to go higher up for the Helium ion. If we try n=4 we have transitions from m=5, 6, 7, etc. The corresponding energys will be: $54.24(\frac{1}{4^2} - \frac{1}{5^2})$=1.22eV, the next one will be: $54.24(\frac{1}{4^2} - \frac{1}{6^2})$=1.8833eV, $54.24(\frac{1}{4^2} - \frac{1}{7^2})$=2.28306V and so on. So these are down to n=4 from level m=6, 7, 8, 9, 10, 11, 12 and 13. The special line a similar analysis gives from m=4 to n=3.

5. Följande antal tillstånd finns för hemoglogin med 0, 1, 2, 3 eller 4 syremolekyler: 1, 4, 6, 4 och 1. Kemiska aktiviteten för O_2 är $\lambda = e^{\mu/\tau}$, ϵ är energin för en bunden O_2. Stora tillstånds summan är $Z = 1 + 4\lambda e^{-\epsilon/\tau} + 6\lambda^2 e^{-2\epsilon/\tau} + 4\lambda^3 e^{-3\epsilon/\tau} + \lambda^4 e^{-4\epsilon/\tau}$. sannolikheten för 1 syremolekyl $P(1) = \frac{4\lambda e^{-\epsilon/\tau}}{Z}$ och sannolikheten för 4 syremolekyler $P(4) = \frac{\lambda^4 e^{-4\epsilon/\tau}}{Z}$. Figuren över $P(1)$ kommer $P(1)$ att uppvisa ett maximum vid något λ och figuren över $P(4)$ kommer $P(4)$ att gå från 0 mot 1 med ökande λ.