LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Quantum Physics F0047T

Examination date: 2019-01-15
The solutions are just suggestions. They may contain several alternative routes.

1. The eigenfunctions of the infinite square well in one dimension are (Here a solution of the S.E. in one dimesion is adequate)

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

In two dimensions the eigenfunctions and eigenenergys are (Here an argument about separation of variables is needed)

$\Psi_{n,m}(x, y) = \psi_n(x) \cdot \psi_m(y)$ and eigenenergys $E_{n,m} = E_n + E_m$ where $n = 1, 2, 3, ..$ and $m = 1, 2, 3, ..$

a) The eigenfunctions inside the square

$$\Psi_{n,m}(x, y) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \cdot \sqrt{\frac{2}{a}} \sin \frac{m\pi y}{a} \quad \text{where} \quad n = 1, 2, 3, .. \text{ and } m = 1, 2, 3, ..$$

The eigenfunctions outside the square $\Psi_{n,m}(x, y) = 0$
b) The four lowest eigenenergys are

$$E_{n,m} = \frac{\pi^2\hbar^2}{2ma^2}(n^2 + m^2), \quad \text{where the 4 lowest are } (n^2 + m^2) = 2, 5, 8, \text{ and } 10.$$

c) The four lowest eigenenergys have degeneracys (either one or two) as follows:

$$E_{1,1} = \text{ one state } (n^2 + m^2 = 2)$$
$$E_{1,2} = E_{2,1} = \text{ two states } (n^2 + m^2 = 5)$$
$$E_{2,2} = \text{ one state } (n^2 + m^2 = 8)$$
$$E_{1,3} = E_{3,1} = \text{ two states } (n^2 + m^2 = 10)$$

2. (a) An appropriate model to use is a **particle in a box** in 1, 2 or 3 dimensions of size $L = 1$ fm$= 1 \cdot 10^{-15}$m. Here a calculation of the 3 dimensional version is made. The eigenenergys of the particle in the box in one dimension are given by:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad \text{where} \quad n = 1, 2, 3, ...$$

and in three dimensions this will become:

$$E_{n_x,n_y,n_z} = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \quad \text{where} \quad n_{x,y,z} = 1, 2, 3, ...$$

Use the ground state to calculate the estimate.

$$E_{1,1,1} = \frac{3\pi^2\hbar^2}{2mL^2} = \frac{3\pi^2(1.054 \cdot 10^{-34})^2}{2 \cdot 9.1094 \cdot 10^{-31} \cdot 1 \cdot 10^{-30} \cdot 1.6022 \cdot 10^{-19}} = 1.13 \cdot 10^{12} \text{ eV} \approx 1 \text{ TeV}$$

Note this is a very high energy !

(b) Another appropriate model you may use is the **spherical box** in 3 dimensions.

(c) Another appropriate model you may use is the **free electron model** and calculate the Fermi energy E_F.

(d) Another appropriate model you may use is the **harmonic oscillator** in 1, 2 or 3 dimensions. This is perhaps not a really good box as the walls are not very hard as the box actually will consist of a parabola. The energy of the ground state in 3 dimensions is

$$E_{0,0,0} = \frac{3}{2}\hbar\omega$$

Now the frequency ω has to be determined. The strenght (and shape of the parabola) is determined by ω. To relate the length scale to ω we can use the an appropriate expectation value for x. $< x >= 0$ cannot be used but $< x^2 >= (n + \frac{1}{2})\frac{\hbar}{m\omega}$ setting $n = 0$ we have $< x^2 >= \frac{1}{2}\frac{\hbar}{m\omega}$. Now we can find an estimate for $< x^2 >= \left(\frac{L}{2}\right)^2 = \frac{1}{4}10^{-30}\mathrm{m}^2$.

$$E_{0,0,0} = \frac{3}{2}\hbar\frac{1}{2}\frac{\hbar}{m < x^2 >} = \frac{3(1.054 \cdot 10^{-34})^2}{4 \cdot 9.1094 \cdot 10^{-31} \cdot 0.25 \cdot 10^{-30} \cdot 1.6022 \cdot 10^{-19}} = 2.28 \cdot 10^{11} \text{ eV}$$

Whatever model one applies the energy will be very high. In the case of the harmonic oscillator also an estimate had to be made for ω. Also the harmonic oscillator does not have as 'hard' walls as the walls of an infinite box. As one can argue for any of these three models an answer in the range of 0.1 - 1 TeV is reasonable.

An electron with a kinetic energy in this range will however also be relativistic.

3. The appropriate spin opperators are

$$S_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ and } S_z = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

a) For S_z the eigenvalues are $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ and the eigenspinors are for the positive eigenvalue $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and for the negative eigenvalue $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. We have to express the given spinor in terms of the eigenspinors to S_z in the following expansion:

$$\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix} = \frac{1+i}{\sqrt{6}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{2}{\sqrt{6}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1+i}{\sqrt{6}}\chi_+ + \frac{2}{\sqrt{6}}\chi_-$$

The probabillities are now just the absolute squares of the coefficients in the expansion above.

The probabillity to get $+\frac{\hbar}{2}$ is $\frac{2}{6} = \frac{1}{3}$

The probabillity to get $-\frac{\hbar}{2}$ is $\frac{4}{6} = \frac{2}{3}$

b) For S_x we have to do some calculations to find the appropriate eigenspinors. The eigenvalue equation is

$$S_x\chi = \lambda\chi \Leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix} \quad (1)$$

We find the eigenvalues from

$$\begin{vmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm\frac{\hbar}{2}$$

The eigenspinors to S_x corresponding to the $+\frac{\hbar}{2}$ we get from

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = +\frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}$$

This gives two identical equations $a = b$. Now let $a = 1$ and hence $b = 1$. This gives the unnormalised spinor

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ and after normalisation we have } \chi_{x+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

For the negative eigenvalue we get the $a = -b$ and hence the eigen spinor is

$$\chi_{x-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Now we have to express the given spinor in terms of the eigenspinors to S_x:

$$\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix}$$

We make use of the projection by operating from the left with χ^*_{x+}:

$$\chi^*_{x+}\chi = \frac{1}{\sqrt{2}}(1 \quad 1) * \frac{1}{\sqrt{6}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix} = \frac{3+i}{\sqrt{12}}$$

For the other spinor we find (operating from the left with χ^*_{x-}):

$$\chi^*_{x-}\chi = \frac{1}{\sqrt{2}}(1 \quad -1) * \frac{1}{\sqrt{6}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix} = \frac{i-1}{\sqrt{12}}$$

Now we know howto expand χ in the eigenspinors of S_x

$$\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix} = \frac{3+i}{\sqrt{12}}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{i-1}{\sqrt{12}}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{3+i}{\sqrt{12}}\cdot\chi_{x+} + \frac{i-1}{\sqrt{12}}\cdot\chi_{x-}$$

The probabillities are now just the absolute squares of the coefficients in the expansion above.

The probabillity to get $+\frac{\hbar}{2}$ is $\frac{10}{12} = \frac{5}{6}$

The probabillity to get $-\frac{\hbar}{2}$ is $\frac{2}{12} = \frac{1}{6}$

4. (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

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

The expectation value of L^2 is

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

5. The Carbon ion has $Z = 6$ and hence the energys levels are $E_n = -\frac{488.16}{n^2}$eV for a carbon ion with just one electron (Hydrogen like). Try to find a start of the series. In order to do that we calculate the energys of the spectral lines. The energy of a spectral line has to be matched to a energy difference between two levels of the Carbon ion. The energy of $\lambda = 207.80$nm is $E = h\nu = \frac{hc}{\lambda} = \frac{6.626 \cdot 10^{-34} \cdot 2.9979 \cdot 10^8}{207.80 \cdot 10^{-9} \cdot 1.6022 \cdot 10^{-19}} = 5.9663$eV . A similar calculation gives the energy for the other lines in the series: 9.56395, 11.8989 and 13.4997 eV.

As the Balmer series in Hydrogen is for transitions down to level n=2 we (see from E_n) have to go higher up in n for the Carbon ion as the energys for a transition to the level $n = 2$ in Carbon would be far to large.

We can solve the problem in two ways either in a sofisticated way or by brute force.

The sofisticated way. Using the fact that can assume levels are adjecent we let n be the quantum number for the lower level and m for a level above, we have no knowledge of how n and m relate. We know however that for the next level (higher in energy) we have down to n from level $m + 1$. One can form the following two equations

$$5.9663eV = 488.16(\frac{1}{n^2} - \frac{1}{m^2})eV \text{ and}$$

$$9.56395eV = 488.16(\frac{1}{n^2} - \frac{1}{(m+1)^2})eV$$

we only need two of the lines to form an appropriate set of equations. (You can use the other pairs of lines as well to form two equations.) Subtracting one equation from the other to

eliminate n you get 3.59765=488.16($\frac{1}{m^2} - \frac{1}{(m+1)^2}$) and finally
$\frac{1}{m^2} - \frac{1}{(m+1)^2} = 0.007369817273025237627$. Solving for m you arrive at $m = 6$. If you do not want to solve the equation above you just try some different values of m untill you find $m = 6$ that solves the equation. Now we use the result for m in 5.9663eV=488.16($\frac{1}{n^2} - \frac{1}{6^2}$)eV to solve for n and we arrive at $n = 5$.

Then there is also the tour of brute force ie just trial and error: If we try n=5 we have transitions from m=6, 7, 8, 9, etc. The corresponding energys will be: 488.16($\frac{1}{5^2} - \frac{1}{6^2}$)=5.97 eV, the next one will be: 488.16($\frac{1}{5^2} - \frac{1}{7^2}$)=9.56 eV, 488.16($\frac{1}{5^2} - \frac{1}{8^2}$)=11.899 eV and so on. So these are down to n=5 from level m=6, 7, 8 and 9.