LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Quantum Physics MTF107

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1. 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.

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

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

   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 coeficient:

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

3. 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 $\frac{\hbar^2}{2I}(l+1)(l+2) - \frac{\hbar^2}{2I} l(l+1) = \frac{\hbar^2}{2I}(l+1), l = 0, 1, 2, 3,$ och detta ger $\frac{\hbar^2}{2I}, 2\frac{\hbar^2}{2I}, 3\frac{\hbar^2}{2I}, 4\frac{\hbar^2}{2I}, ...$
   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
   $\Delta n = -1, \Delta l = -1$: $\hbar\omega + \frac{\hbar^2}{2I}, \hbar\omega + 2\frac{\hbar^2}{2I}, \hbar\omega + 3\frac{\hbar^2}{2I}, \hbar\omega + 4\frac{\hbar^2}{2I}, ...$ Den andra serien har
   $\Delta n = -1, \Delta l = +1$: $\hbar\omega - \frac{\hbar^2}{2I}, \hbar\omega - 2\frac{\hbar^2}{2I}, \hbar\omega - 3\frac{\hbar^2}{2I}, \hbar\omega - 4\frac{\hbar^2}{2I}, ...$

   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
   $R = \sqrt{\frac{h}{4\pi^2 c \Delta\lambda^{-1} \mu}} = 1.30\text{Å}$.

4. Rewrite the wave function in terms of spherical harmonics:

$$\psi(\boldsymbol{r}) = \psi(x,y,z) = N(xy + zy)e^{-\alpha r} = Nr^2 e^{-\alpha r} \left(\frac{1}{i}\sqrt{\frac{2\pi}{15}}(Y_{2,2} - Y_{2,-2}) + \frac{1}{i}\sqrt{\frac{2\pi}{15}}(-Y_{2,1} - Y_{2,-1}) \right)$$

As all the $Y_{l,m}$ have $l = 2$ the probability to get $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$ is one. For L_z we must first normalize the coefficients in front of the $Y_{l,m}$. The sum of the squares is $\frac{8\pi}{15}$ and hence we get the following expression:

$$\psi(\boldsymbol{r}) = Nr^2 e^{-\alpha r} \sqrt{\frac{8\pi}{15}} \left(\frac{1}{i}\sqrt{\frac{1}{4}}(Y_{2,2} - Y_{2,-2}) + \frac{1}{i}\sqrt{\frac{1}{4}}(-Y_{2,1} - Y_{2,-1}) \right)$$

The probability to get $m = 2$ is $|\sqrt{\frac{1}{4}}|^2 = \frac{1}{4}$, for $m = 1$ is $|\sqrt{\frac{1}{4}}|^2 = \frac{1}{4}$, for $m = 0$ is $= 0$ for $m = -1$ is $|\sqrt{\frac{1}{4}}|^2 = \frac{1}{4}$, and for $m = -2$ is $|\sqrt{\frac{1}{4}}|^2 = \frac{1}{4}$

The expectation value $\langle L^2 \rangle = 6\hbar^2$ and for $\langle L_z \rangle = 2\frac{1}{4} + 1\frac{1}{4} + 0 - 1\frac{1}{4} - 2\frac{1}{4} = 0\hbar$.

5. The eigenfunktions of the infinite square well are (Physics handbook)

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

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

$E_n^1 =< H_1 >$ where H_1 is the deviation in the potential from the infinite square well.

$$E_n^1 = \int_0^{a/2} \frac{2\epsilon}{a} \left(1 - \frac{2x}{a}\right) \sin^2 \frac{n\pi x}{a} dx = \left[\text{ change variables } \frac{n\pi x}{a} = y \right] = \int_0^{n\pi/2} \frac{2\epsilon}{n\pi} \left(1 - \frac{2y}{n\pi}\right) \sin^2 y \, dy$$

This can be treated as two separate integrals the first is

$$\int_0^{n\pi/2} \frac{2\epsilon}{n\pi} (1) \sin^2 y \, dy = \frac{2\epsilon}{n\pi} \left[\frac{1}{2} (y - \sin y \cos y)\right]_0^{n\pi/2} = \frac{\epsilon}{n\pi} \left(\frac{n\pi}{2} - \sin \frac{n\pi}{2} \cos \frac{n\pi}{2}\right) = \frac{\epsilon}{2}$$

The second integral is:

$$\int_0^{n\pi/2} \frac{2\epsilon}{n\pi} \left(-\frac{2y}{n\pi}\right) \sin^2 y \, dy = -\frac{4\epsilon}{n^2\pi^2} \int_0^{n\pi/2} \frac{y}{2}(1 - \cos 2y) \, dy =$$

$$-\frac{4\epsilon}{n^2\pi^2} \left[\frac{y^2}{4}\right]_0^{n\pi/2} + \frac{4\epsilon}{n^2\pi^2} \frac{1}{2} \left[\frac{\cos 2y}{4} + \frac{y \sin 2y}{2}\right]_0^{n\pi/2} = -\frac{\epsilon}{4} + \frac{\epsilon}{2n^2\pi^2} [\cos n\pi - 1]$$

Combining the two will give the correction to the unperturbed energies:

$$E_n^1 = \frac{\epsilon}{4} + \frac{\epsilon}{2n^2\pi^2} [(-1)^n - 1]$$

The corrections for n=1 and n=2 are of intrest (**answer to a)**).

$$E_1^1 = \epsilon \left(\frac{1}{4} - \frac{1}{\pi^2}\right) = \epsilon \cdot 0.1486788 = 0.060958\text{eV}, \quad \text{and} \quad E_2^1 = \epsilon \left(\frac{1}{4}\right) = \epsilon \cdot 0.25 = 0.10250\text{eV},$$

The two lowest eigenergies are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{n^2h^2}{8ma^2} \quad [n = 1] \quad E_1 = 6.02465 \cdot 10^{-20}\text{J} = 0.376028\text{eV} \quad \text{and} \quad E_2 = 1.504114\text{eV}$$

The new energys for the two lowest levels are:

$$E_1^* = 0.376028 + 0.060958 = 0.436986\text{eV} \quad \text{and} \quad E_2^* = 1.504114 + 0.04606 = 1.606614\text{eV}$$

And a photon emitted (n=2 to n=1) will have the wavelength (**answer to b)**):

$$\frac{hc}{\lambda} = \Delta E^* = 1.606614 - 0.436986 = 1.169628\text{eV} = 1.87395 \cdot 10^{-19}\text{J} \Rightarrow \lambda = 1.06002 \cdot 10^{-6}\text{m}$$

(If there had been no perturbation it would have been the following:

$$\frac{hc}{\lambda} = \Delta E = 1.504114 - 0.376028 = 1.128086\text{eV} \Rightarrow \lambda = 1.09906 \cdot 10^{-6}\text{m})$$