LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Quantum Physics F0047T

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1. The rotational energy of a molecule is given by

$$E_l = \frac{\hbar^2}{2I} l(l+1)$$

The emitted photon energy for a transition $l+1$ to l is given by

$$E_{photon} = \frac{\hbar^2}{2I}\left((l+1)(l+2) - l(l+1)\right) = \frac{\hbar^2}{2I}\left(l^2 + 3l - 2 - l^2 - l\right) = \frac{\hbar^2(l+1)}{I}$$

This is the energy for one line and there will be a set of lines all for different l. The separation between two adjecent lines in energy will be

$$E_{photon,l+2} - E_{photon,l+1} = \frac{\hbar^2(l+2)}{I} - \frac{\hbar^2(l+1)}{I} = \frac{\hbar^2}{I}$$

The energy of a photon is $E_{photon} = \frac{hc}{\lambda}$ and hence

$$\frac{\hbar^2}{I} = hc\left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2}\right) = 1.2398 \cdot 10^{-6}\left(\Delta\frac{1}{\lambda}\right) \text{eV m} = 1.2398 \cdot 10^{-6} \cdot 20.68 cm^{-1} = 2.564 \cdot 10^{-3}\text{eV}$$

$$I = \frac{(1.055 \cdot 10^{-34})^2}{2.564 \cdot 10^{-3} \cdot 1.602 \cdot 10^{-19}} = 2.71 \cdot 10^{-47}\text{kg m}^2$$

The moment of inertia is $I = mr^2$ where $m = m_H m_{Cl}/(m_H + m_{Cl}) = 35/36 m_H$ and r is the average separation. $r = \sqrt{\frac{I}{m}} = \sqrt{\frac{36 \cdot\ 2.71 \cdot 10^{-47}}{35 \cdot\ 1.673 \cdot 10^{-27}}} = 1.29 \cdot 10^{-10}\text{m}$

$E_l = \frac{2.56 \cdot 10^{-3}}{2} l(l+1)\text{eV}$
$E_0 = 0\text{eV}$,
$E_1 = 2.56 \cdot 10^{-3}\text{eV} = 4.10 \cdot 10^{-22}\text{J}$,
$E_2 = 7.68 \cdot 10^{-3}\text{eV} = 1.23 \cdot 10^{-21}\text{J}$,
$E_3 = 15.4 \cdot 10^{-3}\text{eV} = 2.47 \cdot 10^{-21}\text{J}$,
$E_3 = 25.6 \cdot 10^{-3}\text{eV} = 4.10 \cdot 10^{-21}\text{J}$.

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

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

In three dimensions the eigenfunctions and eigenenergys are (Here an argument about separation of variables is needed to justify the structure of the solution)

$\Psi_{n,m,l}(x, y) = \psi_n(x) \cdot \psi_m(y) \cdot \psi_l(z)$ and eigenenergys $E_{n,m} = E_n + E_m + E_l$ where the indecies are $n = 1, 2, 3, ..$, $m = 1, 2, 3, ..$ and $l = 1, 2, 3, ..$

a) The eigenfunctions inside the box are (note the sidelength is $a/2$ for one of the sides)

$$\Psi_{n,m,l}(x,y,z) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\cdot\sqrt{\frac{2}{a}}\sin\frac{m\pi y}{a}\cdot\sqrt{\frac{4}{a}}\sin\frac{l\pi 2z}{a} \quad \text{where} \quad n=1,2,3,..,m=1,2,3,..\text{ and } \quad l=1,2,3,$$

The eigenfunctions outside the box are $\Psi_{n,m,l}(x,y,z) = 0$

b) The seven lowest eigenenergys are (note the 4 associated to the quantum number l this is due to that the length of the box along the z direction is only half of the other two that are of equal length):

$$E_{n,m,l} = \frac{\pi^2\hbar^2}{2ma^2}(n^2+m^2+4l^2), \quad \text{where the 7 lowest are} \quad (n^2+m^2+4l^2) = 6, 9, 12, 14, 18, \text{ and } 21.$$

c) The seven lowest eigenenergys have degeneracys (different ways to choose n, m, l to form the same energy) (either one, two or four) as follows:

$$E_{1,1,1} = \text{ one state } \ (n^2+m^2+4l^2 = 6)$$

$$E_{1,2,1} = E_{2,1,1} = \text{ two states } \ (n^2+m^2+4l^2 = 9)$$
$$E_{2,2,1} = \text{ one state } \ (n^2+m^2+4l^2 = 12)$$
$$E_{1,3,1} = E_{3,1,1} = \text{ two states } \ (n^2+m^2+4l^2 = 14)$$
$$E_{2,3,1} = E_{3,2,1} = \text{ two states } \ (n^2+m^2+4l^2 = 17)$$
$$E_{1,1,2} = \text{ one state } \ (n^2+m^2+4l^2 = 18)$$

Energy number 7 is special as the degeneracy is 4 but all four are not connected through a symmetry operation, ie some of these states are accidentally degenerated. These four can be grouped in the following way.

$$E_{1,2,2} = E_{2,1,2} = \text{ two states } \ (n^2+m^2+4l^2 = 21)$$

$$E_{1,4,1} = E_{4,1,1} = \text{ two states } \ (n^2+m^2+4l^2 = 21)$$

3. Rewrite $L_x^2 + L_y^2 = L^2 - L_z^2$, which gives the Hamiltonian

$$H = \frac{L^2 - L_z^2}{2\hbar^2} + \frac{L_z^2}{3\hbar^2}.$$

The eigenfunctions are $Y_{l,m}$

$$HY_{l,m} = \left(\frac{L^2 - L_z^2}{2\hbar^2} + \frac{L_z^2}{3\hbar^2}\right)Y_{l,m} = \left(\frac{l(l+1)\hbar^2 - m^2\hbar^2}{2\hbar^2} + \frac{m^2\hbar^2}{3\hbar^2}\right)Y_{l,m}.$$

Hence the energies are:

$$E_{l,m} = \left(\frac{l(l+1)}{2} - \frac{m^2}{6}\right).$$

The lowest (ground state) energy is $E_{0,0} = 0$ ($l = 0$ no rotation).

$l = 1 \to m = 0, \pm 1$, gives $E_{1,0} = 1\text{eV}$ $E_{1,\pm 1} = \frac{5}{6}\text{eV}$

$l = 2 \to m = 0, \pm 1, \pm 2$, gives $E_{2,0} = 3\text{eV}$ $E_{2,\pm 1} = \frac{17}{6}\text{eV}$ $E_{2,\pm 2} = \frac{7}{3}\text{eV}$

and so on.

4. Rewrite the wave function in terms of spherical harmonics: (polar coordinates: $x = r\sin\theta\cos\phi$, $z = r\cos\theta$ and hence $zx = r^2\cos\theta\sin\theta(e^{i\phi}+e^{-i\phi})/2$ using the Euler relations) the appropriate spherical harmonics can now be identified and we arrive at

$$\psi(\boldsymbol{r}) = \psi(x,y,z) = N(zx)e^{-r/3a_0} = N\frac{r^2}{2}\sqrt{\frac{8\pi}{15}}(-Y_{2,1}+Y_{2,-1})e^{-r/3a_0} \ . \tag{1}$$

As all the involved $Y_{l,m}$ have $l = 2$ the probability to get $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$ is one. For the operator L_z we note the two spherical harmonics have the same pre factor (one has -1 and the other has +1 but the absolute value square is the same) ie they will have the same probability. The probability to find $m = 2\hbar$ is 0, for $m = 1\hbar$ is $\frac{1}{2}$, for $m = 0\hbar$ is 0 for $m = -1\hbar$ is $\frac{1}{2}$, and for $m = -2\hbar$ is 0. As all the involved $Y_{l,m}$ have $l = 2$ the probability to get $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$ is one.

b. To calculate the expectation value $<r>$ we need to normalise the given wave function if we wish to do the integral. In order to achieve this in a simple way is to identify the radial wave function. As l is equal to 2 we know that n cannot be equal to 1 or 2 it has to be **larger** or **equal** to 3. By inspection of eq (1) and 2 we find $n = 3$ this function has the correct exponential and the correct power of r (r^2) and hence $R_{3,2}(r) = \frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Z}{3a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$. We also note that $Y_{2,1}$ and $Y_{2,-1}$ are normalised but the sum $(-Y_{2,1}+Y_{2,-1})$ is not normalised. The sum has to be changed to $(-\frac{1}{\sqrt{2}}Y_{2,1}+\frac{1}{\sqrt{2}}Y_{2,-1})$ in order to be normalised. Note that $R_{3,2}(r)$ contains an r^2 term as also a $e^{-r/3a_0}$ term. The wave function can now be completed to the following normalized wave function (note that we do not need to calculate the constant N as all separate parts of $\psi(r)$ are normalised by them selves)

$$\psi(\boldsymbol{r}) = \psi(x,y,z) = N(zx)e^{-r/3a_0} = R_{3,2}(r)(-\frac{1}{\sqrt{2}}Y_{2,1}+\frac{1}{\sqrt{2}}Y_{2,-1})$$

From physics handbook page 292 you find

$$\langle r\rangle = \frac{1}{2}\left[3n^2 - l(l+1)\right]\left(\frac{a_0}{Z}\right) = \frac{1}{2}\left[3\ 3^2 - 2(2+1)\right]\left(\frac{a_0}{1}\right) = \frac{21}{2}a_0 =$$

$$10.5\ \cdot 0.5292\ \text{Å} = 5.56\ \text{Å}.$$

You may also do the integral directly like this:

$$\langle r\rangle = \int_0^\infty\int_0^\pi\int_0^{2\pi} d\phi\ d\theta\ dr\ r^2\sin(\theta)\ r\ \mid R_{3,2}(r)\mid^2 \mid \left(-\frac{1}{\sqrt{2}}Y_{2,1}+\frac{1}{\sqrt{2}}Y_{2,-1}\right)\mid^2 =$$

$$\int_0^\infty dr\ r^3 \mid R_{3,2}(r)\mid^2 = \frac{21}{2}a_0 = 10.5\ \cdot 0.5292\ \text{Å} = 5.56\ \text{Å}.$$

5. (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.