

Q2. We have a particle in a 3D Potential given by $V(r) = \beta r^2 = \beta(x^2 + y^2 + z^2)$

So, TISE reads as

$$\left\{ -\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] + \beta(x^2 + y^2 + z^2) \right\} \psi = E \psi$$

Let's look for separable solutions

$$\psi(x, y, z) = X(x) Y(y) Z(z)$$

Assuming such a solution, TISE reads as

$$-\frac{\hbar^2}{2m} \left[YZ \frac{d^2X}{dx^2} + XZ \frac{d^2Y}{dy^2} + XY \frac{d^2Z}{dz^2} \right] + (\beta x^2 + \beta y^2 + \beta z^2) XYZ = E \cdot XYZ$$

Dividing through by XYZ , we have

$$I \left\{ -\frac{\hbar^2}{2m} \frac{1}{x} \frac{d^2X}{dx^2} + \beta x^2 \right\} \leftarrow \text{only } x \text{-dependence}$$

$$II \left\{ -\frac{\hbar^2}{2m} \frac{1}{y} \frac{d^2Y}{dy^2} + \beta y^2 \right\} = E \leftarrow \text{only } y\text{-dependence}$$

$$III \left\{ -\frac{\hbar^2}{2m} \frac{1}{z} \frac{d^2Z}{dz^2} + \beta z^2 \right\} \leftarrow \text{only } z\text{-dependence}$$

In order for this to hold true for all (x, y, z) , it must be the case that each of I, II, III is individually equal to some constant, say E_x, E_y, E_z resp.

Let us first consider I :

We have

$$-\frac{\hbar^2}{2m} \frac{1}{x} \frac{d^2X}{dx^2} + \beta x^2 = E_x$$

(See next pg.)

Multiplying through by X ,

$$-\frac{\hbar^2}{2m} \frac{d^2X}{dx^2} + \beta x^2 X = E_x X$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \beta x^2 \right] X(x) = E_x X(x). \quad \textcircled{1}$$

This looks just like a 1D QHO! The only difference is, for a 1D QHO, we would have $\beta = \frac{1}{2} m \omega^2$.

We can write $\textcircled{1}$ in terms of \hat{P} and \hat{X} (\hat{X} is the position operator while $X(x)$ is the wavefunction. For now, let's denote wave function $X(x)$ as $\psi(x)$, not to be confused with the overall wavefunction $\Psi(x, y, z)$).

$$\text{as } \left[\frac{1}{2m} \hat{P}^2 + \beta \hat{X}^2 \right] \psi(x) = E \psi(x).$$

let $\beta = \frac{1}{2}mc\omega^2$ with ω being the
 $\Rightarrow \omega = \sqrt{\frac{2\beta}{m}}$ appropriately chosen frequency.

Then, our system in the x -direction is modelled exactly by a 1D QHO.

This is a problem we have already solved! We can use results already obtained!

So, the allowed energies in the x -direction are given by $E_{n_x} = (n_x + \frac{1}{2})\hbar\omega$

and the energy eigenstates are

$$X_{n_x}(x) = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n X_0(x)$$

($X_0(x)$ on next pg)

raising operator, as defined usually.

$$X_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\text{with } \omega = \sqrt{\frac{2B}{m}}$$

Now, the exact same reasoning holds for the y and z directions

Therefore, the Energy of the system is given by

$$E = E_x + E_y + E_z$$

$$\Rightarrow E_{n_x, n_y, n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega$$

where $n_x, n_y, n_z = 0, 1, 2, \dots$

(a). Thus, the **Ground State Energy** of the system, corresponding to $n_x = n_y = n_z = 0$

is

$$E_{000} = \frac{3}{2}\hbar\omega$$

(b). The **Ground State Wavefunction** of the particle is

$$\Psi_{000}(x, y, z) = X_0(x) Y_0(y) Z_0(z)$$

$$\Rightarrow \boxed{\Psi_{000}(x, y, z) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-\frac{m\omega}{2\hbar}(x^2+y^2+z^2)}}$$

with $\omega = \sqrt{\frac{2\beta}{m}}$

(c). To find the degeneracy of the n^{th} level, we want to find the number of pairs (n_x, n_y, n_z) which sum to n .

Using the stars-and-bars method,

$$d(n) = \binom{n+1}{2} = \frac{(n+1)!}{2!(n-1)!}$$

$$\rightarrow \boxed{d(n) = \frac{n(n+1)}{2}}$$

Empty Pg. Couldn't get rid of it.

Q3. The wavefunction Ψ_{nlm} of a Hydrogen atom is given by

$$\Psi_{nlm} = R_{nl}(r) Y_l^m(\theta, \phi)$$

where $Y_l^m(\theta, \phi)$ is a Spherical Harmonic and $R_{nl}(r)$ is the Radial wavefunction, given by

$$R_{nl}(r) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}} e^{-r/na} \left(\frac{2r}{na}\right)^l \left[L_{n-l-1}^{(2l+1)}\left(\frac{2r}{na}\right)\right]$$

So, to find $\Psi_{433}(r, \theta, \phi)$, we want to find the functions

$$R_{43}(r) \quad \text{and} \quad Y_3^3(\theta, \phi).$$

$$Y_l^m(\theta, \phi) = \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!}} e^{im\phi} P_l^m(\cos\theta)$$

$$\Rightarrow Y_3^3(\theta, \phi) = \sqrt{\frac{7}{4\pi} \cdot \frac{1}{6!}} e^{i3\phi} P_3^3(\cos\theta)$$

$$\Rightarrow \boxed{Y_3^3(\theta, \phi) = \sqrt{\frac{35}{64\pi}} e^{i3\phi} \sin^3(\theta)}$$

and

$$L_q^p(x) = (-1)^p \left(\frac{d}{dx} \right)^p L_{p+q}(x).$$

where

$$L_q(x) = \frac{e^x}{q!} \left(\frac{d}{dx} \right)^q (e^{-x} x^q)$$

Thus,

$$L_0^7(x) = (-1)^7 \left(\frac{d}{dx} \right)^7 L_7(x)$$

and

$$L_7(x) = \frac{e^x}{7!} \left(\frac{d}{dx} \right)^7 (e^{-x} x^7).$$

Carrying the appropriate calculations out,
we find that

$$\boxed{L_0^7(x) = 1}$$

Thus, $\boxed{L_0^7\left(\frac{r}{2a}\right) = 1}$

So, the radial wavefunction, $R_{43}(r)$, is

$$\begin{aligned} R_{43}(r) &= \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}} e^{-r/na} \left(\frac{2r}{na}\right)^l [L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)] \\ &= \sqrt{\left(\frac{2}{4a}\right)^3 \frac{(4-3-1)!}{2(4)(4+3)!}} e^{-r/4a} \left(\frac{2r}{4a}\right)^l L_{4-3-1}^{2(3)+1}\left(\frac{2r}{4a}\right) \end{aligned}$$

$$\Rightarrow R_{43}(r) = \sqrt{\frac{1}{(2a)^3} \frac{0!}{8 \times 7!}} e^{-\frac{r}{2a}} \left(\frac{1}{2a}\right)^l \underbrace{L_0^7\left(\frac{r}{2a}\right)}_1$$

$$\Rightarrow R_{43}(r) = \frac{1024 \sqrt{35}}{105 (16a)^{3/2}} \left[\frac{r^3}{(16a)^3} \right] \exp\left(-\frac{4r}{16a}\right)$$

Thus, the wavefunction is

$$\begin{aligned} \Psi_{433}(r, \theta, \phi) &= R_{43}(r) Y_3^3(\theta, \phi) \\ &= \frac{1024 \sqrt{35}}{105 (16a)^{3/2}} \left[\frac{r^3}{(16a)^3} \right] e^{-\frac{4r}{16a}} \\ &\quad \times \sqrt{\frac{35}{64\pi}} e^{i3\phi} \sin^3(\theta) \end{aligned}$$

$$\begin{aligned} \Rightarrow \Psi_{433}(r, \theta, \phi) &= \frac{1024 \times 35}{108 (8\sqrt{\pi})} \cdot \frac{1}{(16a)^{3/2}} \left[\frac{r^3}{(16a)^3} \right] \\ &\quad \times e^{-\frac{4r}{16a}} e^{i3\phi} \times \sin^3(\theta) \end{aligned}$$

$$\Rightarrow \boxed{\Psi_{433}(r, \theta, \phi) = \frac{1}{6144\sqrt{\pi}} \cdot \frac{r^3}{a^{9/2}} \cdot e^{-\frac{r}{4a}} e^{i3\phi} \sin^3(\theta)}$$

(b) - To find the expected value of r in this state, we find

$$\langle r \rangle = \langle \Psi_{433} | r | \Psi_{433} \rangle$$

$$= \int_0^{\pi} \int_0^{2\pi} \int_0^{\infty} \Psi_{433}^*(r, \theta, \phi) r \Psi_{433}(r, \theta, \phi) \cdot r^2 \sin \theta dr d\phi d\theta$$

$$\Rightarrow \langle r \rangle = \frac{1}{(6144)^2 \pi a^9} \int_0^{\pi} \int_0^{2\pi} \int_0^{\infty} \left\{ \left(r^3 e^{-\frac{r}{4a}} e^{i3\phi} \sin^3 \theta \right) r \right\} \\ \times \left\{ \left(r^3 e^{-\frac{r}{4a}} e^{i3\phi} \sin^3 \theta \right) \right\} r^2 \sin \theta dr d\phi d\theta$$

$$\Rightarrow \langle r \rangle = \frac{1}{(6144)^2 \pi a^9} \int_0^{\pi} \int_0^{2\pi} \int_0^{\infty} r^9 e^{-\frac{r}{2a}} \sin^7(\theta) dr d\phi d\theta$$

$$= \frac{1}{(6144)^2 \pi a^9} \times (2\pi) \times \int_0^{\infty} r^9 e^{-\frac{r}{2a}} dr \times \int_0^{\pi} \sin^7(\theta) d\theta$$

$$\text{Let } I_1 = \int_0^{\pi} \sin^7(\theta) d\theta.$$

$$\text{Then } I_1 = \int_0^{\pi} (\sin^6 \theta) \sin \theta d\theta$$

$$= \int_0^{\pi} (1 - \cos^2 \theta)^3 \sin \theta d\theta$$

$$\text{Let } u = \cos \theta \Rightarrow du = -\sin \theta d\theta$$

$$\begin{aligned} \text{When } \theta = 0, u &= 1 \\ \theta = \pi, u &= -1 \end{aligned}$$

$$\Rightarrow I_1 = \int_{-1}^1 (1 - u^2)^3 du$$

$$\begin{aligned} (1 - u^2)^3 &= (1 - u^2)(1 - u^2)(1 - u^2) \\ &= (1 - u^2) + (-u^2 + u^4) + (-u^2 + u^4) \\ &\quad + (u^4 - u^6) \end{aligned}$$

$$\Rightarrow I_1 = \int_{-1}^1 (1 - 3u^2 + 2u^4 - u^6) du$$

This is easy to calculate, and we get

$$\boxed{I_1 = \frac{32}{35}}$$

$$\text{Next, let } I_2 = \int_0^\infty r^9 e^{-r/2a} dr$$

$$\begin{aligned} \text{Let } \frac{r}{2a} &= t \Rightarrow r = t(2a) \\ &\Rightarrow dr = 2a dt \end{aligned}$$

$$\begin{aligned} \text{When } r &= 0, t = 0 \\ r &= \infty, t = \infty. \end{aligned}$$

$$\text{Thus, } I_2 = (2a)^{10} \int_0^\infty t^9 e^{-t} dt$$

At this point, I gave up and used an Integral Calculator:

$$I_2 = (2a)^{10} \times 362880$$

$$\text{So, } \langle r \rangle = \frac{2}{6144^2 a^9} \times I_1 \times I_2$$

$$= \frac{2}{6144^2 a^9} \times \frac{32}{35} \times (2a)^{10} \times 362880$$

$\Rightarrow \langle r \rangle = 18a$, where a is the Bohr Radius

$$(c). \text{ Now, } \hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$\text{So, } \hat{L}_x^2 + \hat{L}_y^2 = \hat{L}^2 - \hat{L}_z^2$$

and since $[\hat{L}, \hat{L}_z] = 0$, we can measure definite values for \hat{L}, \hat{L}_z simultaneously.

- $\hat{L}|n, l, m\rangle = \hbar l(l+1)|n, l, m\rangle$
- $\hat{L}_z|n, l, m\rangle = \hbar m|n, l, m\rangle$

$$\text{So, } \hat{L}\psi_{433} = \hbar 3(3+1)\psi_{433}$$

$$\hat{L}_z\psi_{433} = \hbar 3\psi_{433}$$

So, if we were to measure $(\hat{L}_x + \hat{L}_y)$, we would get

$$(\hat{L}_x + \hat{L}_y) \Psi_{433}(r, \theta, \phi) = (\hat{L} - \hat{L}_z) \Psi_{433}(r, \theta, \phi)$$

$$= 3(4)\hbar \Psi_{433}(r, \theta, \phi) - 3\hbar \Psi_{433}(r, \theta, \phi)$$

$$\Rightarrow (\hat{L}_x + \hat{L}_y) \Psi_{433}(r, \theta, \phi) = 3\hbar \Psi_{433}(r, \theta, \phi)$$

Thus, if we were to measure the quantity $(L_x + L_y)$ of the state $\Psi_{433}(r, \theta, \phi)$, we would obtain the value $3\hbar$.
