# Quantum Mechanics Week 5: Class Activities solutions

Q1)

By matching with the eigenfunctions of the hydrogen atom, we find $(n, l, m) = (2,1,0)$.

The corresponding values of energy, total angular momentum and the $z$-component of angular momentum are then:

$$E = \frac{E_1}{n^2} = \frac{E_1}{4}$$
$$L^2 = l(l+1)\hbar^2 = 2\hbar^2$$
$$L_z = m\hbar = 0$$

Q2)

The wavefunction satisfies the normalisation relation in spherical polar co-ordinates,

$$\int_0^\infty dr \int_0^{2\pi} d\phi \int_0^\pi d\theta \;\, r^2 \sin\theta \, |\psi|^2 = 1$$

With $\psi = N \cos\theta \;\, r \, e^{-r/2a}$, we have

$$N^2 \int_0^\infty r^4 \, e^{-\frac{r}{a}} \, dr \int_0^{2\pi} d\phi \int_0^\pi \cos^2\theta \sin\theta \, d\theta = 1$$
$$\rightarrow N^2 \cdot \left( a^5 \int_0^\infty u^4 \, e^{-u} \, du \right) \cdot (2\pi) \cdot \left( \left[ -\frac{1}{3} \cos^3\theta \right]_0^\pi \right) = 1$$
$$\rightarrow N^2 \cdot 24a^5 \cdot 2\pi \cdot \frac{2}{3} = 1$$
$$\rightarrow N = \sqrt{\frac{1}{32\pi}} \cdot \frac{1}{a^{5/2}}$$

Q3)

There are 3 other eigenfunctions with the same energy, i.e. with $n = 2$. Their quantum numbers are $(n, l, m) = (2,0,0)$, $(2,1,1)$ and $(2,1,-1)$.

Q4) The radial probability density is given by:

$$P(r) \propto r^2 R(r)^2 \propto r^4 e^{-r/a}$$

This peaks where $\frac{dP}{dr} = 0$, or $\frac{d}{dr}\left(r^4 e^{-r/a}\right) = \left(4r^3 - \frac{r^4}{a}\right) e^{-r/a} = 0$. Hence, the probability peaks where $r = 4a$.

Q5) The expectation value can be found by:

$$\langle r \rangle = \int_0^\infty r\, P(r)\, dr = \frac{1}{24a^5}\int_0^\infty r^5\, e^{-r/a}\, dr = \frac{1}{24}a\int_0^\infty u^5\, e^{-u}\, du = 5a$$

This does not agree with the answer to part e), but this is fine because the mean and peak of a function can be different.

Q6) Substituting $\psi(x,y,z) = f(x)\, g(y)\, h(z)$ into the 3D Schrödinger equation

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

and using $V = 0$, we have

$$-\frac{\hbar^2}{2m}\left(g(y)\, h(z)\frac{d^2 f(x)}{dx^2} + f(x)\, h(z)\frac{d^2 g(y)}{dy^2} + f(x)\, g(y)\frac{d^2 h(z)}{dz^2}\right) = E\, f(x)\, g(y)\, h(z)$$

Dividing all terms by $f(x)\, g(y)\, h(z)$, we find:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{f(x)}\frac{d^2 f}{dx^2} + \frac{1}{g(y)}\frac{d^2 g}{dy^2} + \frac{1}{h(z)}\frac{d^2 h}{dz^2}\right] = E$$

Q7) The solution for each co-ordinate looks like, for example:

$$-\frac{\hbar^2}{2m}\frac{1}{f(x)}\frac{d^2 f}{dx^2} = E_x$$
$$\rightarrow -\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2} = E_x f$$

This is the same as the 1D Schrödinger equation for the infinite potential well, such that we already know that the energy eigenvalues are

$$E_x = \frac{\pi^2\hbar^2}{8mL^2}(n_x^2)$$

where $n_x$ is an integer. Using these solutions back in the solution for Q6 we have,

$$E = E_x + E_y + E_z = \frac{\pi^2\hbar^2}{8mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

Q8) 54 is a sum of 3 squares in 3 possible ways:

$$1^2 + 2^2 + 7^2 = 54$$
$$2^2 + 5^2 + 5^2 = 54$$
$$3^2 + 3^2 + 6^2 = 54$$

$\left(n_x, n_y, n_z\right) = (1,2,7)$ can be re-arranged in 6 possible permutations, and $\left(n_x, n_y, n_z\right) =$ (2,5,5) and (3,3,6) can be re-arranged in 3 possible permutations. Listing them all out:

| $n_x$ | $n_y$ | $n_z$ |
|---|---|---|
| 1 | 2 | 7 |

| | | |
|---|---|---|
| 1 | 7 | 2 |
| 2 | 1 | 7 |
| 2 | 7 | 1 |
| 7 | 1 | 2 |
| 7 | 2 | 1 |
| 2 | 5 | 5 |
| 5 | 2 | 5 |
| 5 | 5 | 2 |
| 3 | 3 | 6 |
| 3 | 6 | 3 |
| 6 | 3 | 3 |