Quantum Mechanics Week 5: Class Activities

We'll go through these activities in Wednesday's Week 5 Quantum Mechanics tutorial.

Warm-up discussion

- Check the solution methods for the 3D Schrödinger equation for a central potential
- Quantum numbers of the hydrogen atom

Wavefunctions of the hydrogen atom!

1) An electron in an energy eigenfunction of the hydrogen atom has a wavefunction given by:

$$\psi(r,\theta,\phi) = N \cos\theta \; r \, e^{-r/2a}$$

where a is the Bohr radius. What are the values of the quantum numbers (n,l,m) in this case, and the corresponding values of the energy (as a fraction of the ground-state energy), total angular momentum and z-component of angular momentum of the electron?

2) Derive the value of the normalisation constant N of the wavefunction given in part b). [*Hint:* $\int_0^\infty u^n \, e^{-u} \, du = n!$ *where n is an integer.]*

3) How many other eigenfunctions ψ_{nlm} have the same energy as the eigenfunction given in Q1, and what are their corresponding quantum numbers?

Finding the most likely radial co-ordinate of the electron

4) Write down an expression for the probability density of finding the electron with wavefunction given in Q1 as a function of radius r. At what value of r does this probability peak?

5) Determine the expectation value of the radial co-ordinate of the electron with wavefunction given in Q1. Does this answer agree with your answer to Q4? If not, explain why.

If you have time and want to try something …

Consider a particle in a 3D box with co-ordinates (x,y,z), defined by potential

$$V(x,y,z) = \begin{cases} 0, & |x| < L, |y| < L, |z| < L \\ \infty, & \text{otherwise} \end{cases}$$

6) Substitute a trial separable solution $\psi(x, y, z) = f(x)\, g(y)\, h(z)$ into the 3D Schrödinger equation, and hence show that in the region where $V = 0$,

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

7) Each term on the left-hand side of the above equation depends on only 1 variable, but each of these variables is independent – so the only way this equality can hold as (x, y, z) varies is if each term on the left-hand side is separately equal to a constant. Use this reasoning to show that $f(x)$, $g(y)$ and $h(z)$ must all be solutions of the 1D infinite potential well, and

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

where (n_x, n_y, n_z) are integers.

8) How many distinct eigenfunctions of the cubical box have energy $\frac{\pi^2 \hbar^2}{8mL^2} \times 54$ (i.e., have $n_x^2 + n_y^2 + n_z^2 = 54$)? (These are known as degenerate quantum states.)

The rest of this week's activities

Please complete the Week 5 Online Quiz (10 multiple choice questions) by the end of Sunday. Each Online Quiz represents 1% of the unit grade.

Assignment 2: You can now solve Q2 in Assignment 2 (which is due at the end of Friday Week 6).