

Atomic Spectrum of Hydrogen:

- The emission spectrum of hydrogen is composed of discrete wavelengths, giving evidence that the gaps between energy levels are fixed.
- That atomic visible line spectra of hydrogen fall into series had been known since Balmer showed that they followed; $\frac{1}{\lambda} = R(\frac{1}{n^2} - \frac{1}{2^2})$ where R is a constant.
- This measures the energy it takes from an electron to move from one energy state to the next.
- The hydrogen atom has a set of allowed energies given by; $E_n = -E_r(\frac{1}{n^2})$ where $n = 1, 2, 3, \dots$ and R is the Rydberg constant at $2.18 \times 10^{-18} \text{ J}$.

Allowed Energies of the Hydrogen Atom:

- The lowest allowed energy is E_1 , Rydberg constant and as n increases, E_n approaches the energy of an unbound electron, or 0.
- The potential energy function for a nucleus of atomic number Z is; $V(r) = -Ze^2/r$.
- The allowed energies now become; $E_n = E_r(\frac{Z^2}{n^2})$.
- The energy of bound states lowered by increased attraction of more highly charged nucleus.

The Bohr Atom:

- Neils Bohr developed a quantum model of a single electron near a hydrogen nucleus.
- He postulated a set of circular orbits for electrons with specific, discrete radii and energies and that electrons could move in each orbit without radiating energy.

Quantum Theory and Matter Waves:

- In quantum theory, mass and energy are not distinguished, with matter such as electrons behaving like a wave and energy such as radiation behaving like a particle.
- $\lambda = \frac{h}{p} = \frac{h}{mv}$ where p is momentum, m is the mass, v is the velocity and h is the Planck constant.

Lecture 6: Properties of Waves and Shapes of Electron Atomic Orbitals:

Electrons Resist being confined:

- An electron confined between two walls adopts a minimum energy waveform with wavelength twice the distance between the walls.
- Electrons are waves in three dimensions.

There is a Minimum Energy Waveform:

- Electrons don't fall right down into the nucleus because they have a wavelength which \neq zero.
- For hydrogen atoms, it is peaked in the middle with $E = -E_r$.

The lowest energy waveform has no nodes:

- The minimum energy (frequency) waveform has no nodes and when amplitude zero, it's a node.
- Subsequent higher energy waveforms have nodes, and the more nodes means a shorter wavelength, more momentum and thus higher energy. $p = h/\lambda$.

Waves in 2D – the Drumhead:

- The higher-order harmonic oscillations in higher dimensions also have nodes where the drumhead never moves, and the nodes are lines in the plane of the circumference of the drum.
- The quantum description of a bound electron is simply a standing wave in three dimensions.

The 1s Wave function:

- The lowest energy ($n=1$) waveform for the hydrogen atom corresponds to one, spherically symmetric, wave function. $\psi^{\circ} = e(-r)$.
- Called the 1s orbital, corresponding to an energy $E_1 = -E_r = -2.18 \times 10^{-18} \text{ J}$.

The 1s Orbital:

- This orbital can be represented as a radial function, as gradient/contour, or simply as a lobe
- The pluses and minus just refer to opposite sides of the waves.

Lobe Representation:

- Because electrons aren't bound, the radial part of all wave functions decays exponentially.
- Lobes are commonly drawn to represent surfaces of constant electron density.
- Nodes are when there is zero probability of finding an electron.

The 2s (principal quantum number) Orbital:

- Higher energy wave functions have more nodes and shorter wavelengths.
- As we increase principal quantum number, number of spherical nodes/axis crosses increases.
- The relationship between n (principal quantum number), is that there is $n - 1$ nodes.

The Born Interpretation:

- Born postulated that the electron density is proportional to the square of the wavefunction (ψ^2).
- ψ^2 is always positive so this removes the complication of the sign of the amplitude of the wave.
- Higher energy, & higher quantum number, electron wavefunctions extend further from nucleus.

Lecture 7: P and D Orbitals:

Waves in 2D – The Drumhead:

- Higher order harmonic oscillations have nodes & the + - refers to when the wave is up or down.
- The nodes are lines in the plan of the circumference of the drum; *1s = 1 circular, 2s = 2 circular.*
- A linear node in 2D translates to a planar node, & there are three orientated along the xyz axes.
- Lowest energy p-orbital has a node, ascribed principal quantum no. $n = 2$ and denoted *2p orbital.*
- Adding spherical nodes increase n , but keep general shape; *3p = 1 planar and 1 spherical node.*

Orbital Angular Momentum:

- Electrons bound orbitals have angular momentum because if not moving in circular orbital then distance from the centre is changing and so angular momentum exists.
- *For $n = 1, L = 0$ – Only an s orbital. For $n = 2, L = 0$ (s orbital) or 1 (p orbitals).*
- The only thing that changes angular momentum is a planar mode.