

The Bohr model of the H atom (1913)

- Explains the hydrogen atomic emission spectrum by using the idea of quantization
- **Postulates:**
 - The electron travels around the nucleus in **circular orbits** without loss of energy
 - The angular momentum of the electron is quantized → **only certain orbits are allowed**
- **Consequences:**
 - The energy of the H atom is quantized → only certain **discrete energy levels** (stationary states) are allowed
 - Each circular orbit corresponds to one **E-level**

• Consequences (cont.):

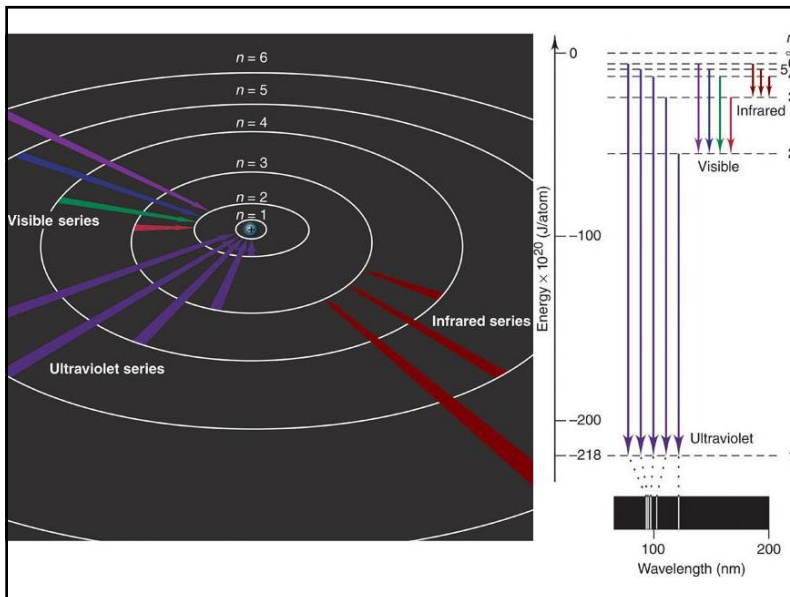
- A transition between two energy states generates a **photon** with energy equal to the difference between the two levels (ΔE)

$$E_{ph} = E_{state\ 2} - E_{state\ 1} = h\nu \Rightarrow \Delta E = h\nu$$

- A photon with a specific (discrete) frequency is emitted for each transition from a higher to a lower **E-level**

⇒ Atomic emission spectra consist of discrete lines

- Each orbit is labeled with a number, **n**, starting from the orbit closest to the nucleus ($n = 1, 2, \dots$)
- The same number is used to label the energy levels → **n** is the **quantum number**



• Energy states of the H atom

$$E_n = -B \left(\frac{Z^2}{n^2} \right) \quad n = 1, 2, 3, \dots, \infty$$

B is a constant ($B = 2.18 \times 10^{-18} \text{ J}$)

Z is the nuclear charge (For H: $Z = 1 \rightarrow E_n = -B/n^2$)

- **Ground state** – the lowest energy state ($n = 1$)

$$E_1 = -B/1^2 = -B = -2.18 \times 10^{-18} \text{ J}$$

- **Excited states** – higher energy levels ($n > 1$)

- The energy increases with increasing **n**
- The highest possible energy is for $n = \infty$ (the electron is completely separated from the nucleus)

$$E_\infty = -B/\infty^2 = 0$$

- A transition between two E -levels with quantum numbers n_1 and n_2 will produce a photon with energy equal to the E -difference between the levels, ΔE :

$$\Delta E = E_{n_2} - E_{n_1} = \left(-\frac{B}{n_2^2} \right) - \left(-\frac{B}{n_1^2} \right) = B \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$$\Delta E = E_{ph} = h\nu = \frac{hc}{\lambda} = B \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$$\Rightarrow \frac{1}{\lambda} = \frac{B}{hc} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \leftarrow \text{Rydberg eq.} \left(\frac{B}{hc} = R \right)$$

- **Ionization energy (I)** of the H atom – the energy needed to completely remove the electron from a H atom in its ground state (can be viewed as the energy change from E_1 to E_∞)

$$\Delta E = E_\infty - E_1 = \left(-\frac{B}{\infty^2} \right) - \left(-\frac{B}{1^2} \right) = 0 - (-B) = B$$

$$\Rightarrow I = B = 2.18 \times 10^{-18} \text{ J/atom}$$

• Limitations of the Bohr Model

- Applicable only to **H-like** atoms and ions (having a single electron) in the absence of strong electric or magnetic fields (H, He⁺, Li²⁺, ...)

7.3 The Wave-Particle Duality of Matter and Energy

- **Mass-energy equivalency** (Einstein)

$$E = mc^2$$

- For a photon with energy $E = h\nu = hc/\lambda$:

$$E = mc^2 = hc/\lambda \Rightarrow mc = h/\lambda \Rightarrow \lambda = h/mc$$

$$\Rightarrow \lambda = h/p \quad p - \text{photon momentum}$$

- The equation shows that the wave-like photons have particle-like mass and momentum

- Experimental evidence (Compton, 1923)

- **De Broglie's hypothesis** (1924) – all matter has wave-like properties (just as waves have particle-like properties)

- For a particle with mass, m , and velocity, u , the wavelength is:

$$\lambda = h/mu$$

- De Broglie's equation is equivalent to that for a photon ($\lambda = h/mc$)
- De Broglie's equation combines particle properties (m, u) with wave properties (λ)

\Rightarrow Matter and energy exhibit wave-particle duality

- **Example:** Calculate the wavelengths of an electron ($m = 9.109 \times 10^{-31} \text{ kg}$) with velocity $2.2 \times 10^6 \text{ m/s}$ and a bullet ($m = 5.0 \text{ g}$) traveling at $700. \text{ m/s}$.

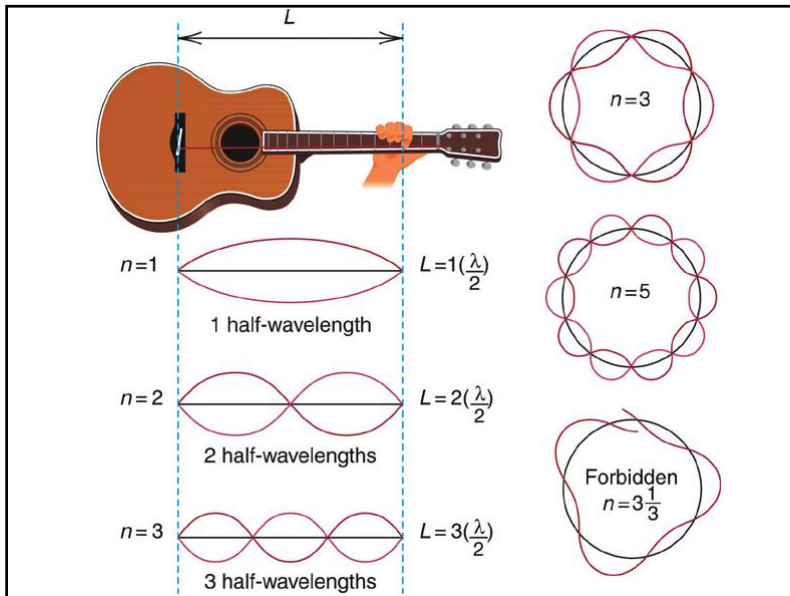
$$\lambda(e^-) = \frac{h}{mu} = \frac{6.626 \times 10^{-34} \text{ J} \cdot \text{s}}{9.109 \times 10^{-31} \text{ kg} \times 2.2 \times 10^6 \text{ m/s}}$$

$$= 3.3 \times 10^{-10} \text{ m} = 0.33 \text{ nm} \rightarrow \text{comparable to atomic sizes}$$

$$\lambda(\text{bul}) = \frac{h}{mu} = \frac{6.626 \times 10^{-34} \text{ J} \cdot \text{s}}{5.0 \times 10^{-3} \text{ kg} \times 700. \text{ m/s}}$$

$$= 1.9 \times 10^{-34} \text{ m} \rightarrow \text{very short, undetectable}$$

- **Experimental evidence** (Davisson and Germer, 1927)
 - **Diffraction of electrons** by crystal surfaces
 - Diffraction patterns are consistent with the wavelength predicted by de Broglie's relation
- The electron can be treated as a wave with a very short wavelength (similar to the wavelength of x-rays)
- The electron confined in the **H** atom can be treated as a **standing wave** having discrete frequencies (energies) like a guitar string



- **Heisenberg's uncertainty principle** (1927) – the exact position and momentum (velocity) of a particle can not be known simultaneously

$$\Delta x \cdot \Delta p \geq h/4\pi$$

Δx and $\Delta p = m\Delta u$ – uncertainty in position and momentum, respectively

- A consequence of the wave-particle duality of matter
- The exact location of very small particles is not well known due to their wave-like properties
- The probability to find a particle at a particular location depends on the amplitude (intensity) of the wave at this location