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 ($\Delta E$)
  \[ E_{ph} = E_{state\ 2} - E_{state\ 1} = h\nu \implies \Delta E = h\nu \]
- A photon with a specific (discrete) frequency is emitted for each transition from a higher to a lower $E$-level
  \[ \implies \text{Atomic emission spectra consist of discrete lines} \]
  - Each orbit is labeled with a number, $n$, starting from the orbit closest to the nucleus ($n = 1, 2, \ldots$)
  - The same number is used to label the energy levels → $n$ is the quantum number

**Energy states of the H atom**

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

$B$ is a constant ($B = 2.18\times10^{-18}$ J)

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

- **Ground state** – the lowest energy state ($n = 1$)
  \[ E_1 = -B/1^2 = -B = -2.18\times10^{-18} \text{ J} \]

- **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, $\Delta E$:

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

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

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

• 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 $E_\infty$)

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

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

• 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 $E = h\nu = hc/\lambda$:
  $$E = mc^2 = \frac{hc}{\lambda} \Rightarrow mc = \frac{h}{\lambda} \Rightarrow \lambda = \frac{h}{mc}$$

$$\Rightarrow \lambda = \frac{h}{p} \quad p \quad \text{– photon momentum}$$
  – 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:
  $$\lambda = \frac{h}{mu}$$
  – De Broglie’s equation is equivalent to that for a photon ($\lambda = \frac{h}{mc}$)
  – De Broglie’s equation combines particle properties ($m, u$) with wave properties ($\lambda$)

$$\Rightarrow \text{Matter and energy exhibit wave-particle duality}$$
• **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. \(\text{m/s}\).

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

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

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

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

• **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

\[\Delta x \cdot \Delta p \geq \frac{h}{4\pi}\]

\[\Delta x and \Delta p = m\Delta u\] – 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