

Schrödinger's Theory and Heisenberg's uncertainty principle

'Electron in a box' model:

- ▶ Imagine an electron confined to a box (sides of length L)
- ▶ If you treat the electron as a wave, the wavelength is:

$$\lambda = \frac{h}{p}$$

- ▶ If it is assumed that:
 - ▶ The electron can only be found along that linear length
 - ▶ And: the electron cannot escape from the box
- ▶ A logical conclusion is that the electron wave is 0 at the edge of the box and the electron is a standing wave in the box.

▶

Electron energy and momentum:

- ▶ Wavelength is related to the length of the box:

$$\lambda = \frac{2L}{n} \quad (\text{n is an integer})$$

- ▶ Therefore, momentum of the electron is:

$$p = \frac{nh}{2L}$$

- ▶ And its kinetic energy is:

$$E_k = \frac{p^2}{2m} = \frac{n^2 h^2}{8mL^2}$$

- ▶ Where n is an integer representing the energy level;
 h = Planck's constant L = length of the box
 and m = mass of an electron

▶

Therefore...

- ▶ Because our electron is confined to a box, then we conclude that the energy of the electron is discrete ('quantized')
- ▶ NOT a perfect (or very realistic) model, but it allows us to see that there are discrete sets of energies for electrons
- ▶ AND—paved the way for Schrödinger...



Review of Schrödinger's theory:

- ▶ Every electron is associated with a particular wavefunction (similar to de Broglie)
- ▶ A wavefunction is a function of the position (x) and the time (t) for the electron
- ▶ Total energy of an electron "in a box" is given by the following equation:

$$E = -\frac{C}{n^2}$$
 - ▶ Where C is a constant and n is the energy level of the electron
 - ▶ m = mass of the electron
 - ▶ e = charge of the electron
 - ▶ h = Planck's constant
 - ▶ k = Coulomb constant
$$C = \frac{2\pi^2 m e^4 k^2}{h^2}$$



Which results in...

$$E = -\frac{13.6}{n^2}$$

- ▶ Where the units are in electronvolts
- ▶ Schrödinger theory also helps explain the atomic spectra and why there are variations in the spectral intensities
 - ▶ Because the calculations of energy are based on probabilities...
- ▶ Example: Calculate the wavelength of the photon emitted in the transition from energy level n = 3 to n = 2 for a Hydrogen atom.



Example answer:

$$E_3 = -\frac{13.6}{3^2} = -1.51eV$$

$$E_2 = -\frac{13.6}{2^2} = -3.40eV$$

$$E_3 - E_2 = 1.89eV$$


