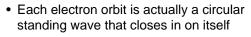


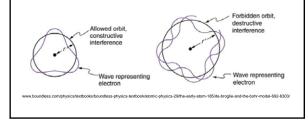
Electrons as Waves

- de Broglie's hypothesis of electron waves provide an explanation for Bohr's theory of the hydrogen atom
- A particle of mass *m* moving with speed *v* would have a wavelength of

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



• If the wave does not close in on itself, then destructive interference takes place and the wave quickly dies out



• The only waves that persist are those for which the circumference of the orbit has a whole number of wavelengths

_

• So for an orbit of radius r

$$2\pi r = n\lambda$$
$$2\pi r = \frac{nh}{mv}$$
$$mvr = \frac{nh}{2\pi}$$

- The electron is not oscillating in a circular wave, but rather the wave pattern represents the amplitude of the electron wave
- But Bohr's model does not work for atoms other than hydrogen
- · A new theory was needed
- That new theory is called quantum mechanics

The Schrödinger Theory

- Erwin Schrödinger (1926) provided a realistic, quantum model for the behavior of electrons in atoms
- There is a wave associated with the electron called the **wavefunction**, $\psi(x,t)$, and is a function of position *x* and time *t*

• Given the forces acting on the electron, the wave function can be determined by solving the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)$$

or the simplified 1 dimensional form

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial t^2}$$

- The wavefunction is not directly observable but its amplitude is significant
- The square of the amplitude of the wavefunction is proportional to the probability per unit volume of finding the particle (called probability density)

 $P(r) = \left|\Psi\right|^2 \Delta V$

The Heisenberg Uncertainty Principle

- Werner Heisenberg (1927)
- The principle applied to position and momentum states that it is not possible to measure simultaneously the position **and** momentum of something with indefinite precision
- This has nothing to do with imperfect measuring devices or experimental error
- If represents a fundamental property of nature

• The uncertainty Δx in position and the uncertainty Δp in momentum are related by

$$\Delta x \Delta p \ge \frac{h}{4\pi}$$

- This says that making momentum as accurate as possible makes position inaccurate, whereas accuracy in position results in inaccuracy in momentum
- If one is made zero, the other has to be infinite
- The uncertainty principle also applies to measurements of energy and time
- If a state is measured to have energy *E* with uncertainty *∆E*, then there must be an uncertainty *∆t* in the time during which the measurement is made, such that

$$\Delta E \Delta t \ge \frac{h}{4\pi}$$

Quantum Tunnelling

- According to classical mechanics, if a particle with energy *E* approaches a barrier with energy U_0 , then the particle will only be able to pass the barrier if $E>U_0$
- However, the wavefunction associated with the particle must be continuous at the barrier and will show an exponential decay through the barrier

The wavefunction must also be continuous on the other side of the barrier so there is a probability that the particle will tunnel through the barrier.



- As a particle approaches the barrier, it is described by a free particle wave function
- When it reaches the barrier, it must satisfy the Schrodinger equation in the form

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2} = (E - U_0)\Psi(x)$$

• Which has the solution

$$\Psi = A e^{-\alpha x} \qquad \text{where} \qquad \alpha = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

