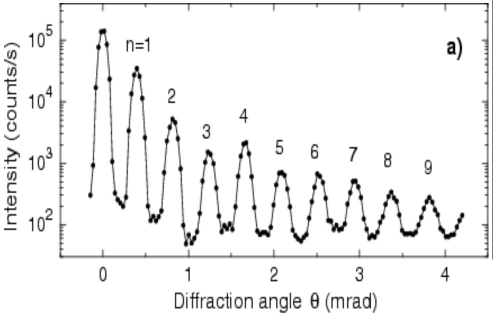
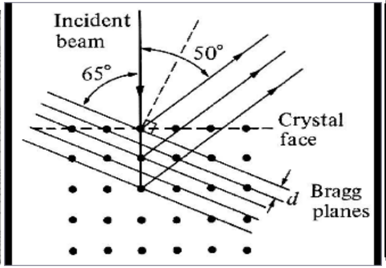
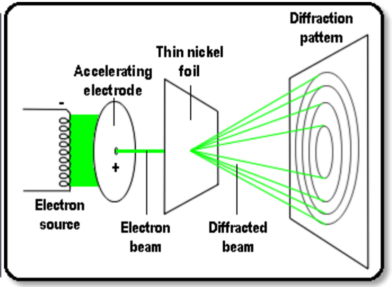
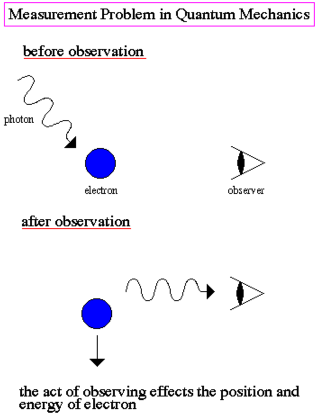
Wave Nature of Matter

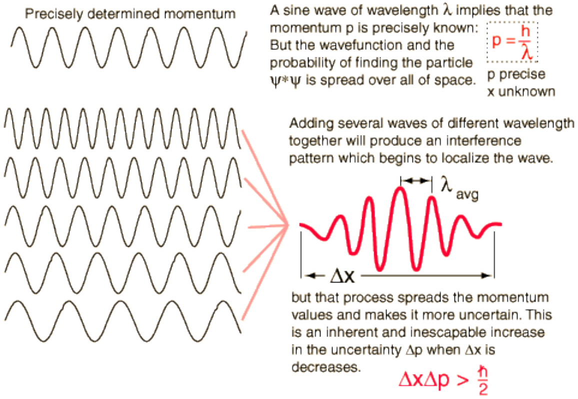






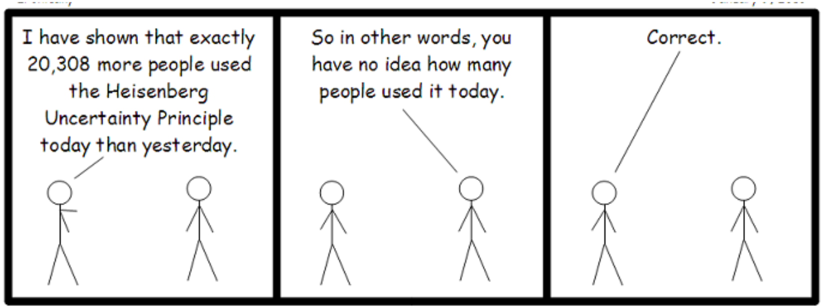
Uncertainty Principle

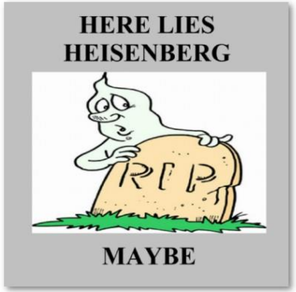




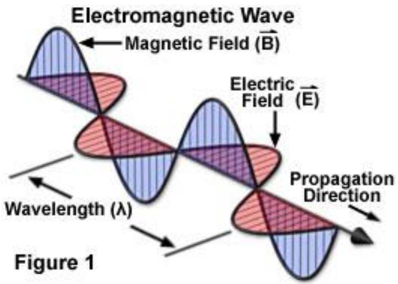
Uncertainty principle

$$\Delta x . \Delta p_x \geq \frac{h}{4\pi}$$





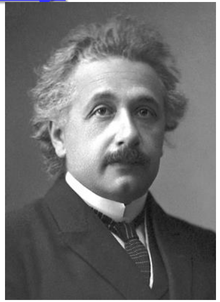
Photoelectric Effect: Wave –Particle Duality

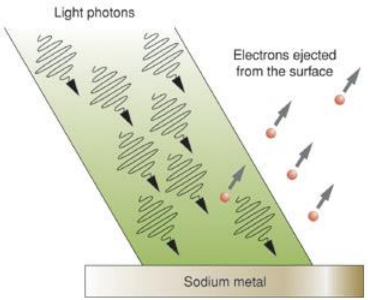


Electromagnetic Radiation

$E = E_0 Sin(kx - \omega t)$

Wave energy is related to Intensity
I $\propto E^2{}_o$ and is independent of ω



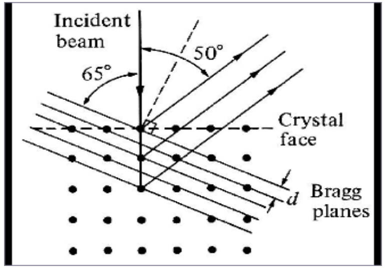


Einstein borrowed Planck's idea that ΔE=hν and proposed that radiation itself existed as small packets of energy (Quanta)now known as PHOTONS

$$E_P = h\nu = KE_M + \phi = \frac{1}{2}mv^2 + \phi$$

ϕ = Energy required to remove electron from surface

Diffraction of Electrons : Wave –Particle Duality



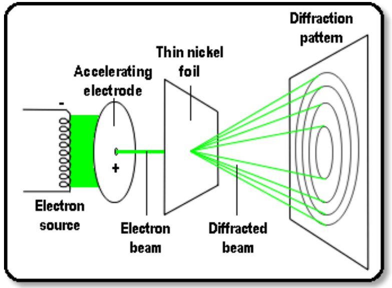
Davisson-Germer Experiment

A beam of electrons is directed onto the surface of a nickel crystal. Electrons are scattered, and are detected by means of a detector that can be rotated through an angle $\boldsymbol{\theta}$. When the Bragg condition $\boldsymbol{m\lambda = 2d\sin\theta}$ was satisfied (d is the distance between the nickel atom, and m an integer) constructive interference produces peaks of high intensity

Diffraction of Electrons : Wave –Particle Duality

G. P. Thomson Experiment

Electrons from an electron source were accelerated towards a positive electrode into which was drilled a small hole. The resulting narrow beam of electrons was directed towards a thin film of nickel. The lattice of nickel atoms acted as a diffraction grating, producing a typical diffraction pattern on a screen



de Broglie Hypothesis: Mater waves

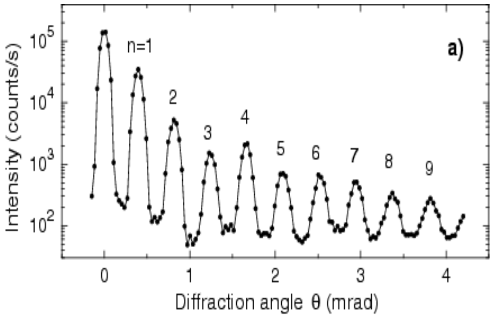
Since **Nature** likes **symmetry,**
Particles also should have **wave-like** nature

De Broglie wavelength

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

Electron moving @ 10^6 m/s

$$\lambda = \frac{h}{mv} = \frac{6.6\text{x}10^{-34}\ \text{J s}}{9.1\text{x}10^{-31}\ \text{Kg} \times 1\text{x}10^{6}\ \text{m/s}} = 7\times10^{-10}\,m$$

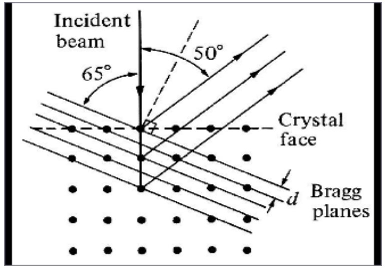


He-atom scattering

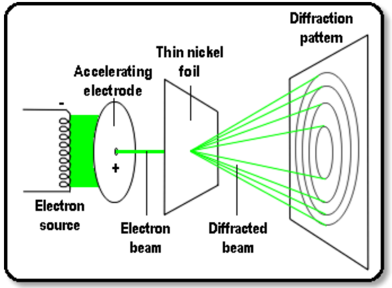
Diffraction pattern of He atoms at the speed 2347 m s^{-1} on a silicon nitride transmission grating with 1000 lines per millimeter. Calculated de Broglie wavelength $42.5\text{x}10^{-12}$ m

de Broglie wavelength too small for macroscopic objects

Diffraction of Electrons : Wave –Particle Duality



The wavelength of the electrons was calculated, and found to be in close agreement with that expected from the De Broglie equation



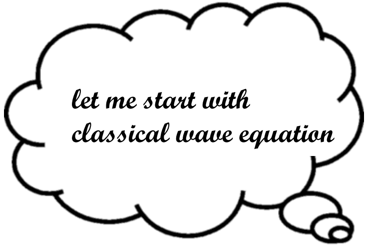
Schrodinger's philosophy

PARTICLES can be **WAVES**
and **WAVES** can be
PARTICLES

- New theory is required to explain the behavior of electrons, atoms and molecules
- Should be Probabilistic, not deterministic
- (non-Newtonian) in nature
- Wavelike equation for describing sub/atomic systems

Schrodinger's philosophy

PARTICLES can be WAVES
and WAVES can be
PARTICLES

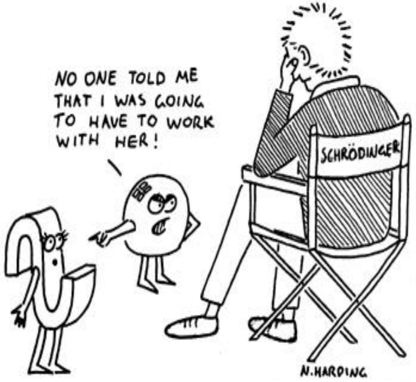


A concoction of

$$E = T + V = \frac{1}{2}mv^2 + V = \frac{p^2}{2m} + V$$

$E = h\nu = \hbar\omega$ Wave is Particle

$\lambda = \frac{h}{p} = \hbar k$ Particle is Wave



Schrodinger's philosophy

$$\frac{\partial^2\Psi(x,t)}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2\Psi(x,t)}{\partial t^2}$$ Classical Wave Equation

$\Psi(x,t) = \text{Amplitude}$

$\Psi(x,t) = Ce^{i\alpha}$; Where $\alpha = 2\pi\left(\frac{x}{\lambda} - \nu t\right)$ is the phase

Remember!

$E = h\nu = \hbar\omega$

$\lambda = \frac{h}{p} = \frac{2\pi}{k}$

$$\alpha = 2\pi\left(\frac{x}{\lambda} - \nu t\right) = \frac{x \cdot p - E \cdot t}{\hbar}$$

Schrodinger Equation

Time-dependent Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\widehat{H}\cdot\Psi(x,t)=\left[\frac{-\hbar^2}{2m}\nabla^2+V(x)\right]\Psi(x,t)$$

$$\widehat{H}\cdot\Psi(x,y,z,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,y,z,t)\ ;\quad \widehat{H}=\frac{-\hbar^2}{2m}\nabla^2+V(x,y,z)$$

Schrodinger equation in 3-dimensions

Schrodinger Equation

Time-dependent Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\widehat{H}\cdot\Psi(x,t)=\left[\frac{-\hbar^2}{2m}\nabla^2+V(x)\right]\Psi(x,t)$$

$$\widehat{H}\cdot\Psi(x,y,z,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,y,z,t)\ ;\quad \widehat{H}=\frac{-\hbar^2}{2m}\nabla^2+V(x,y,z)$$

$$\boxed{\Psi(x,y,z,t)=\psi(x,y,z)\cdot\phi(t)}\Rightarrow\quad \Psi=\psi\cdot\phi$$

$$\widehat{H}\cdot\Psi=i\hbar\frac{\partial}{\partial t}\Psi$$

$$\widehat{H}(\psi\cdot\phi)=i\hbar\frac{\partial}{\partial t}(\psi\cdot\phi)$$

Schrodinger Equation

$$\widehat{H}(\psi\cdot\phi)=i\hbar\frac{\partial}{\partial t}(\psi\cdot\phi)$$

$\widehat{H}$ operates only on ψ and $\dfrac{\partial}{\partial t}$ operates only on ϕ

$$\phi\cdot\widehat{H}\psi=\psi\left(i\hbar\frac{\partial}{\partial t}\phi\right)$$

Divide by $\psi\cdot\phi$

$$\frac{\widehat{H}\psi}{\psi}=\frac{1}{\phi}\left(i\hbar\frac{\partial}{\partial t}\phi\right)$$

LHS is a function of co-ordinates and RHS is function of time. If these two have to be equal then both functions must be equal to constant, say W

Schrodinger Equation

$$\frac{\widehat{H}\psi}{\psi} = \frac{1}{\phi}\left(i\hbar\frac{\partial}{\partial t}\phi\right) = W$$

$$\frac{\widehat{H}\cdot\psi}{\psi} = W \qquad\qquad \widehat{H}\psi = W\psi$$

$$\frac{1}{\phi}\left(i\hbar\frac{\partial}{\partial t}\phi\right) = W \qquad\qquad i\hbar\frac{\partial}{\partial t}\phi = W\phi$$

Separation of variables

The solution of the differential equation

$i\hbar\frac{\partial}{\partial t}\phi = W\phi$ is $\phi(t) = e^{-iWt/\hbar}$

Schrodinger Equation

In classical mechanics $\hat{H}$ represents total energy

We can therefore write

$$\widehat{H}\psi = W\psi \qquad \text{as} \qquad \widehat{H}\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\cdot\psi(x)$$

Schrodinger equation is an eigenvalue equation

There can be many solutions $\boldsymbol{\psi_n(x)}$ each corresponding to different energy $\boldsymbol{E_n}$

Laws of Quantum Mechanics

The mathematical description of Quantum mechanics is built upon the concept of an operator

Classical Variable	QM Operator
Position, x	$\hat{x}$
Momentum, $p_x = mv$	$\hat{p}_x = \frac{\hbar}{i}\frac{d}{dx} = -i\hbar\frac{d}{dx}$
Kinetic Energy, $T_x = \frac{p_x^2}{2m}$	$\hat{T}_x = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$
Kinetic Energy, $T = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$	$\hat{T} = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$
Potential Energy, $V(x)$	$\hat{V}(x)$

Laws of Quantum Mechanics

The values which come up as result of an experiment are the eigenvalues of the appropriate operator

In any measurement of observable associated with operator $\hat{A}$, the only values that will be ever observed are the eigenvalues an, which satisfy the eigenvalue equation:

$$\hat{A} \cdot \Psi_n = a_n \cdot \Psi_n$$

$\boldsymbol{\Psi_n}$ are the eigenfunctions of the system and $\boldsymbol{a_n}$ are corresponding eigenvalues

If the system is in state $\boldsymbol{\Psi_k}$, a measurement on the system will yield an eigenvalue $\boldsymbol{a_k}$