EARLY 20TH CENTURY

Theory of Black body radiation (Planck 1900)

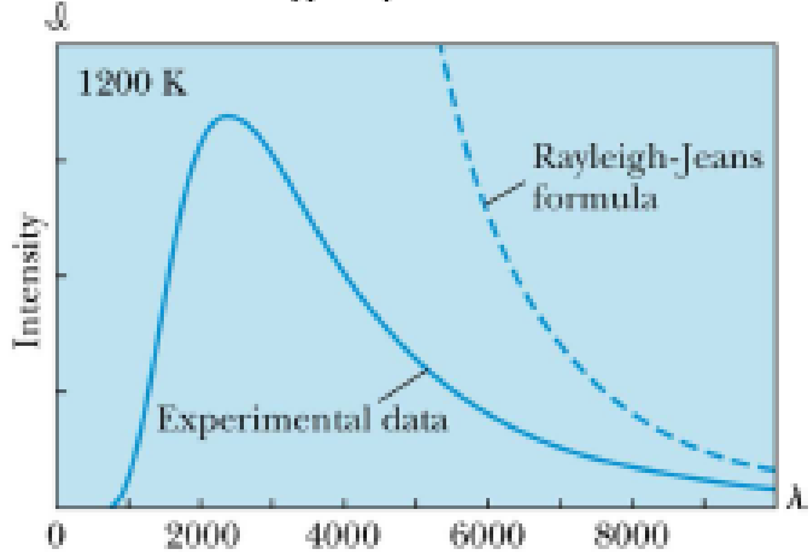
Photoelectric effect (Einstein 1904)

Atomic Structure and Spectroscopy (Bohr 1913)

Compton effect (Compton 1920)

Understanding the blackbody radiation spectrum

- Attempts to fit the low and high wavelength part of the spectrum
- Using classical theory of electromagnetism and thermodynamics, Lord Rayleigh comes up with: $\mathcal{I}(\lambda,T)=\frac{2\pi ckT}{\lambda^4}$ Rayleigh-Jeans formula
- Major flaw at short wavelength ("Ultraviolet catastrophe")



Describing the blackbody emission spectra:
one of the outstanding problems at the beginning of the 20th century

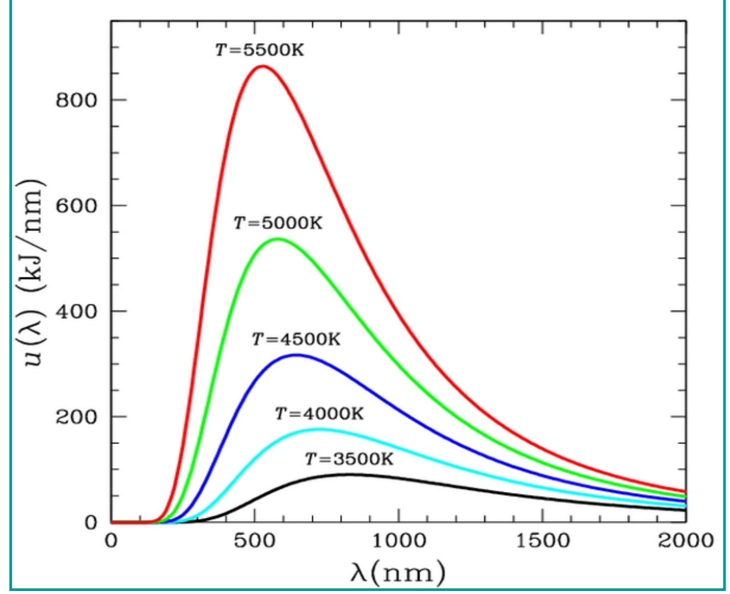
Planck's law of black body radiation (1900) and Quanta of Energy

Planck's assumption (1900):
Radiation of a given frequency ν could only be emitted and absorbed in "quanta" (discrete bundles) of energy

$$E=h\nu$$

h= Planck's constant =6.626×10^{-34} Jsec

ν: frequency of radiation



$$u_\nu d\nu = \frac{8\pi\nu^2}{c^3}\frac{h\nu}{e^{h\nu/K_BT}-1}d\nu$$

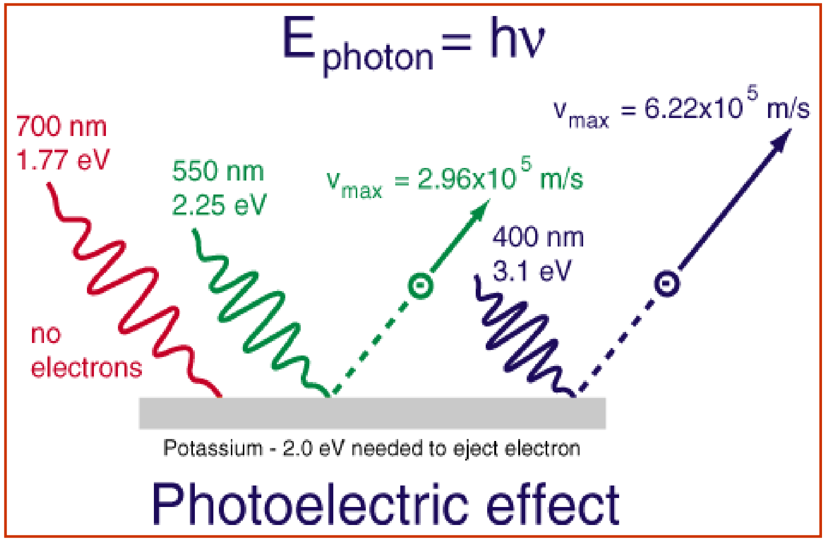
Photo Electric Effect:

In **1839**, ***Alexandre Edmond Becquerel*** observed the photoelectric effect via an electrode in a conductive solution exposed to light.

In **1887**, ***Heinrich Hertz*** made observations of the photoelectric effect and of the production and reception of electromagnetic (EM) waves.

In **1901**, ***Nikola Tesla*** received the U.S. Patent 685957 (Apparatus for the Utilization of Radiant Energy) that describes radiation charging and discharging conductors by "radiant energy".

In **1902**, ***Philipp von Lenard* (N)** observed the variation in electron energy with light frequency.



$$\frac{1}{2}m_e v_k^2 = E_k = h\nu - W$$

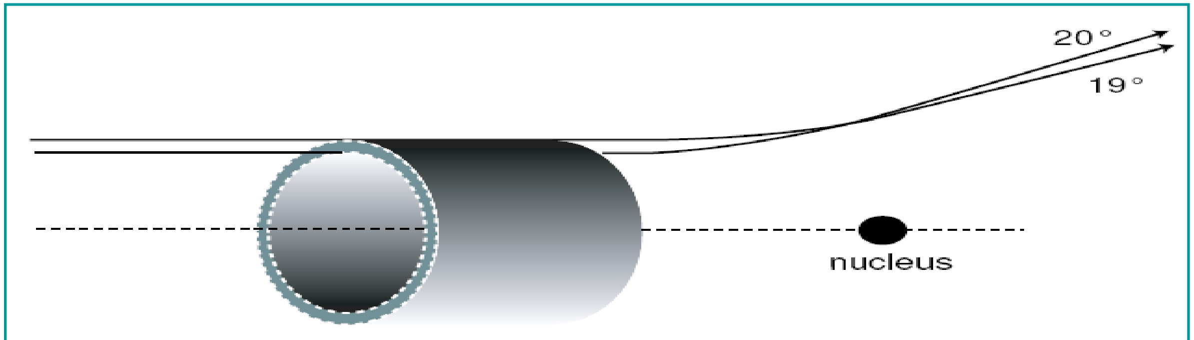
In **1905**, ***Albert Einstein* (N)** proposed the well-known Einstein's equation for photoelectric effect.

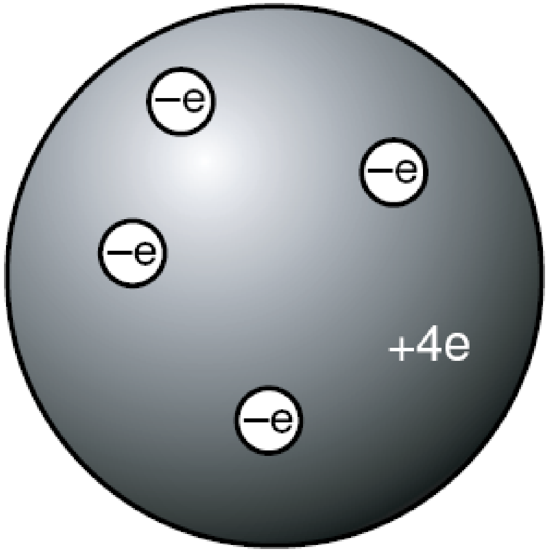
In **1916**, ***Robert Andrews Millikan* (N)** confirms Einstein’s explanation of photoelectric effect.

This shows that Light behaves as particles with quanta of energy

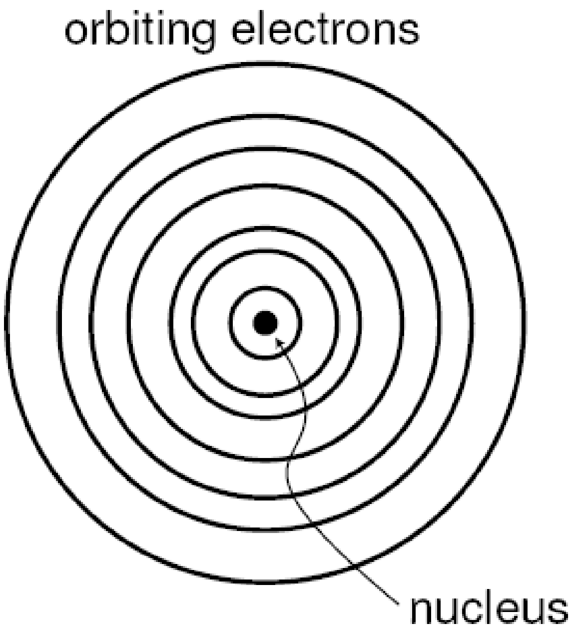
$$E=h\nu$$

Atomic Structure





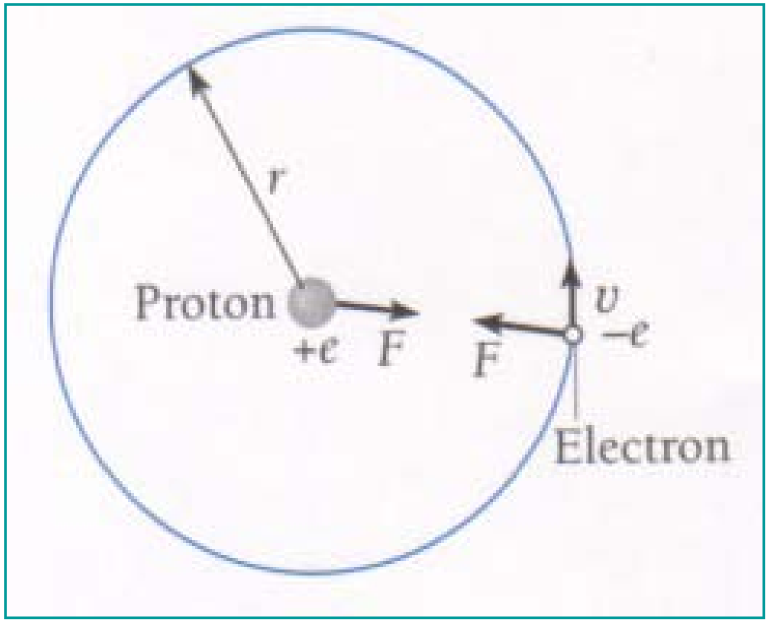
l / The raisin cookie model of the atom with four units of charge, which we now know to be beryllium.



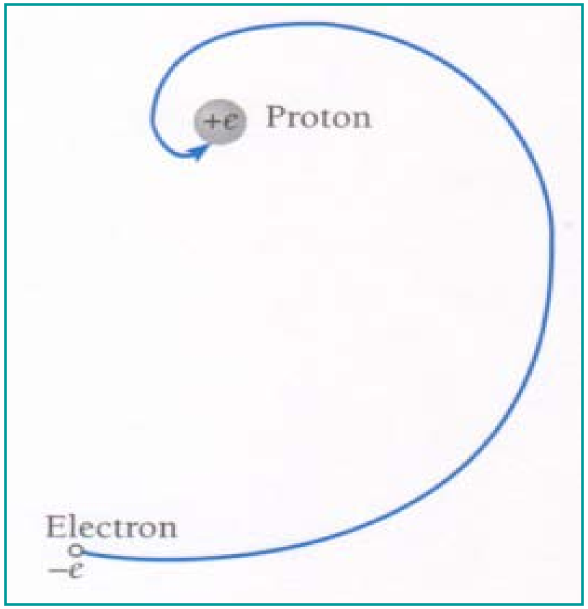
h / The planetary model of the atom.

Nuclear atom model **(1911):**
Ernest Rutherford

Classical physics: atoms should collapse!



This means an electron should fall into the nucleus.



<u>Classical Electrodynamics:</u> charged particles radiate EM energy (photons) when their velocity vector changes (e.g. they accelerate).

New mechanics is needed!

Spectroscopy

from n ≥ 3 to n = 2

Balmer series **(1885)**

visible spectrum

Rydberg formula for hydrogen **(1888)**

$$\frac{1}{\lambda_{\mathrm{vac}}} = R_{\mathrm{H}} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Rydberg formula for all hydrogen-like atom **(1888)**

$$\frac{1}{\lambda_{\mathrm{vac}}} = RZ^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Bohr's formula **(1913)**

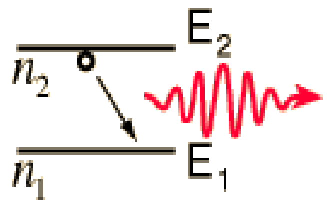
$$\frac{1}{\lambda} = R_{\mathrm{H}} \left(\frac{1}{2^2} - \frac{1}{n^2} \right), n = 3, 4, 5, \ldots$$

Old Quantum Theory

Niels Henrik David Bohr, model of atomic structure, 1913

The electron's *orbital angular momentum* is *quantized*

$$\mathbf{L} = n \cdot \hbar = n \cdot \frac{h}{2\pi}$$



A downward transition involves emission of a photon of energy:

$$E_{photon} = h\upsilon = E_2 - E_1$$

Given the expression for the energies of the hydrogen electron states:

$$h\upsilon = \frac{2\pi^2 m e^4}{h^2}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] = -13.6\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]\text{eV}$$

Electrons travel in discrete orbits around the atom's nucleus.
The chemical properties of the element being largely determined by the number of electrons in each of the outer orbits

$$E_n = \frac{-13.6\ \text{eV}}{n^2} \qquad = \frac{-m_e q_e^4}{8h^2\epsilon_0^2}\frac{1}{n^2}$$

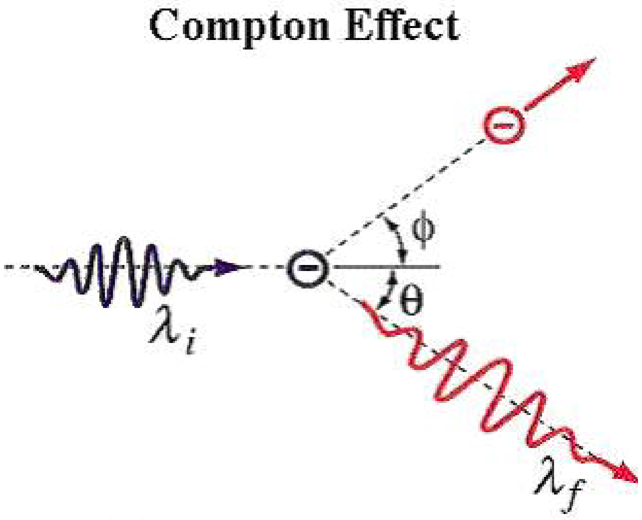
$$E = E_i - E_f = \frac{m_e e^4}{8h^2\epsilon_0^2}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

$$\frac{1}{\lambda} = \frac{m_e e^4}{8ch^3\epsilon_0^2}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

Energy and Momentum of Photons

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

$$P = \hbar k = \frac{h}{\lambda} \qquad \hbar = \frac{h}{2\pi}$$



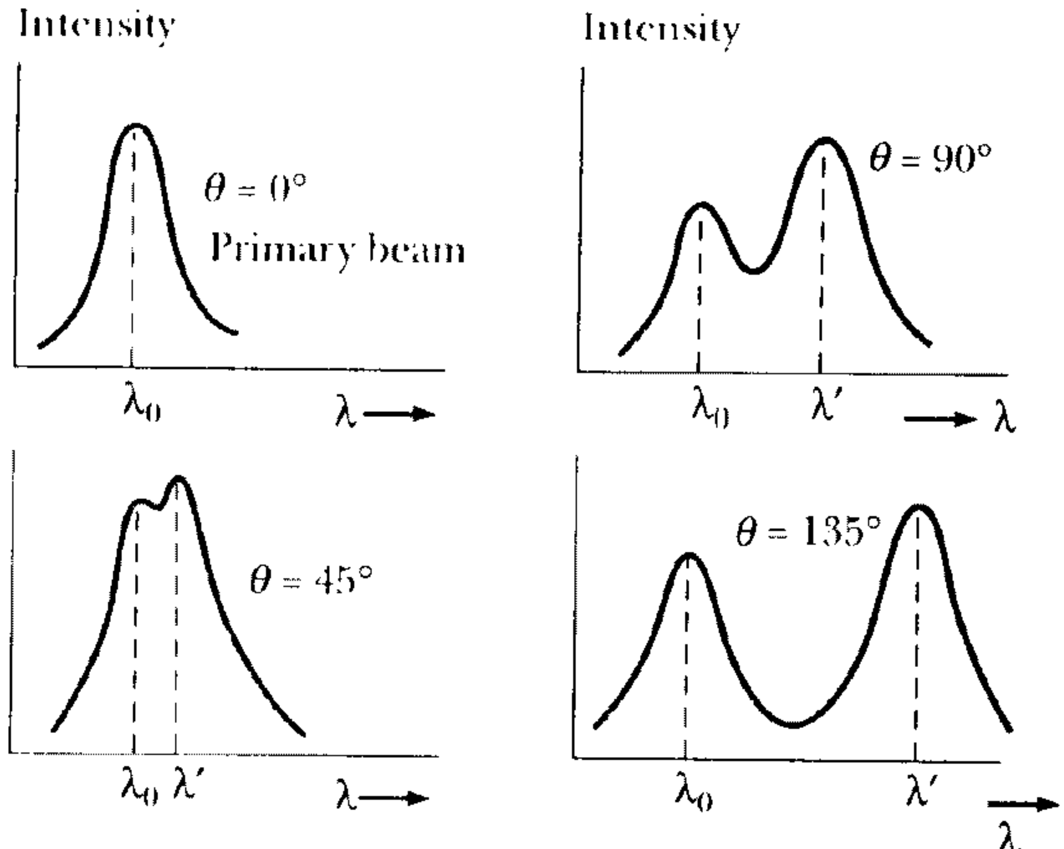
Shift in wavelength of the scattered photon in Compton Scattering

$$\Delta\lambda = \frac{h}{mc}(1-\cos\theta)$$

Compton wavelength

$$\lambda_c = \frac{h}{mc}$$

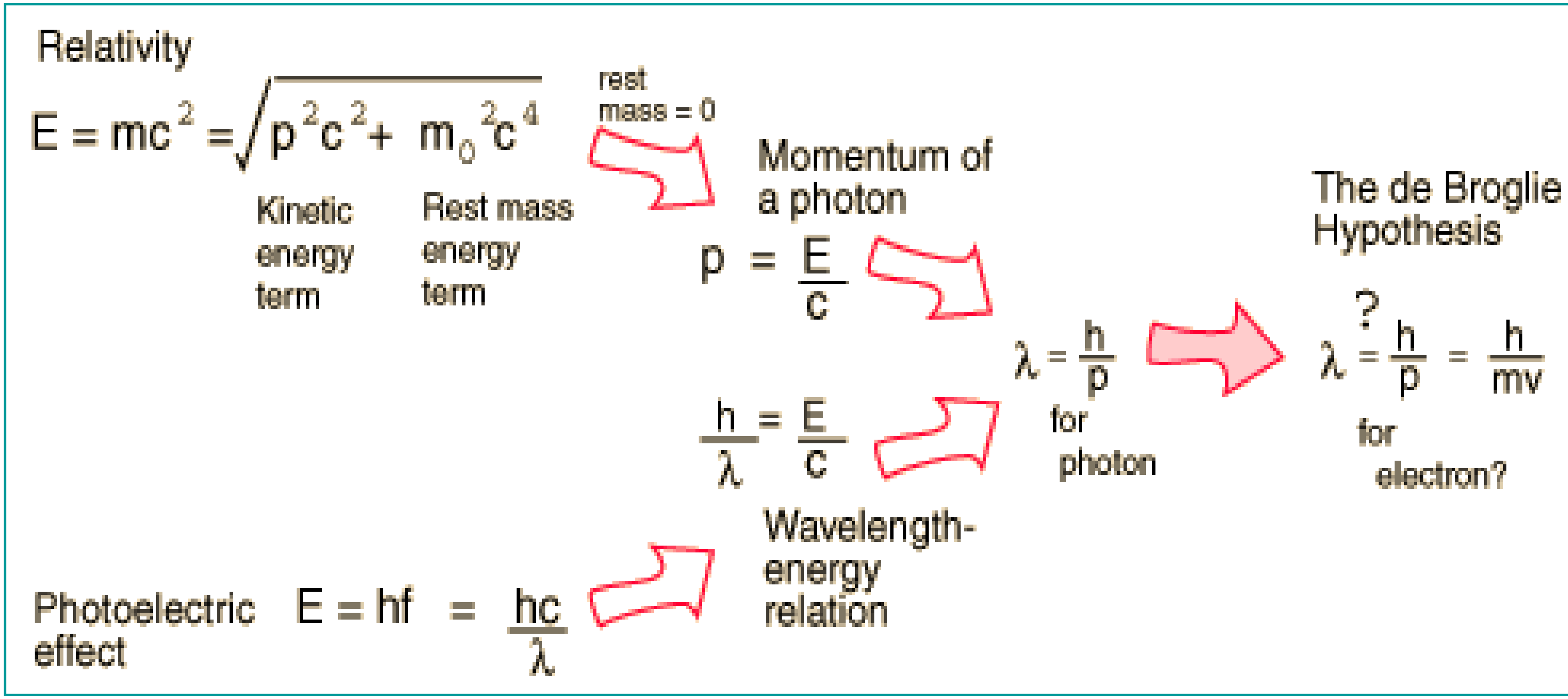
$$= 2.4\times10^{-12}\,m$$



(b)

de Broglie *matter wave hypothesis* (1923):

All matter has a wave-like nature (*wave-particle duality*) and that the wavelength and momentum of a particle are related by a simple equation.



Phase velocity, Group velocity and velocity of the particles

$$\lambda = \frac{h}{p} \qquad \text{or} \qquad p = \frac{hk}{2\pi} = \hbar k$$

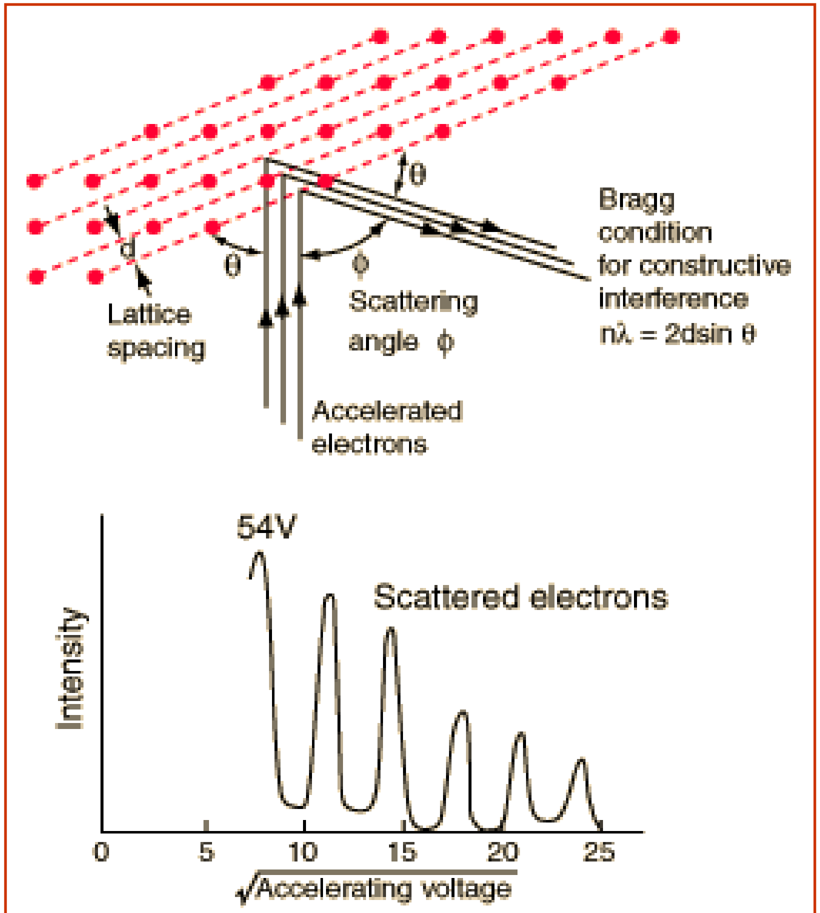
$$E = h\nu = \hbar\omega = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m}$$

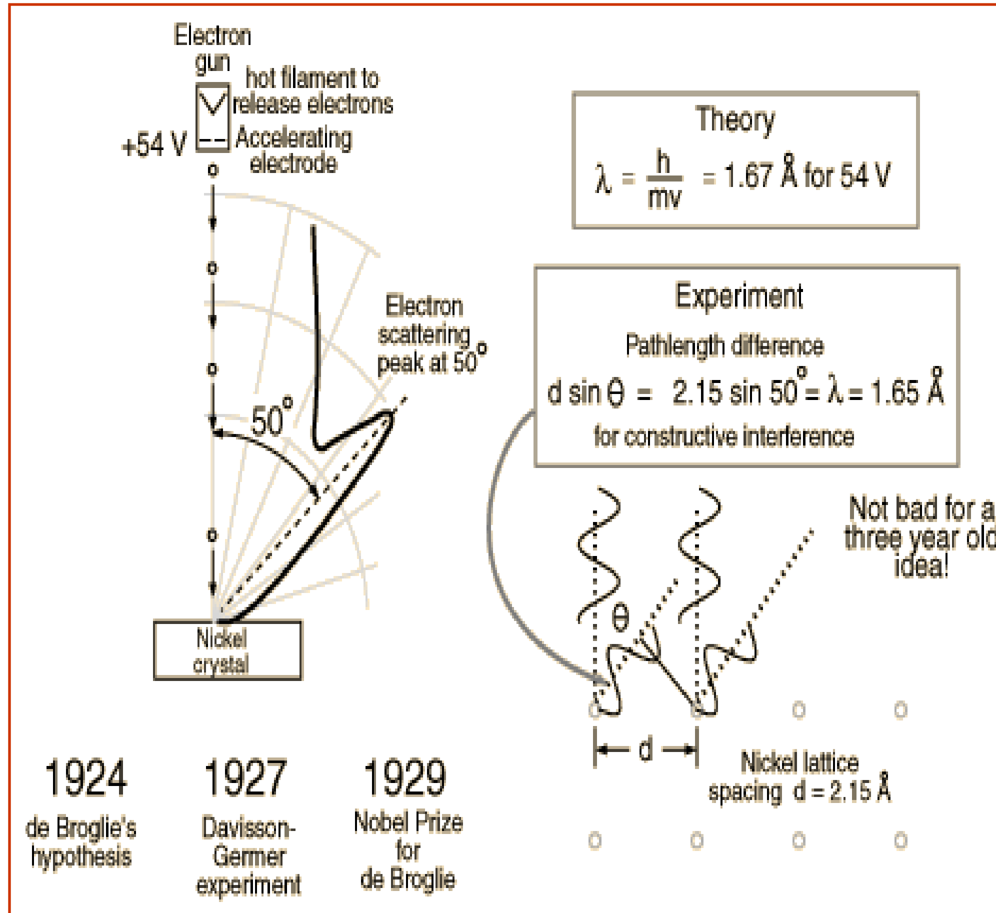
$$\text{Phase velocity:} \qquad v_p = \frac{\omega}{k} = \frac{hk}{4m\pi} = \frac{p}{2m} = \frac{v}{2}$$

$$\text{Group velocity:} \quad v_g = \frac{d\omega}{dk} = \frac{hk}{2\pi m} = 2v_p = v$$

Group velocity v_g is same as the particle velocity v

Davisson-Germer Experiment (1927)





Electron has wave nature (diffraction)!

De Broglie wavelength of electron for $v_e=6x10^6$ m/s:
Distance at which wave nature is prominent

$$h = 6.62\times10^{-34}\,Js; \qquad m_e = 9.1\times10^{-31}\,kg; \qquad J = Nm = kg(m/s)^2$$

$$\text{de Broglie wavelength}: \qquad \lambda_e = \frac{h}{p} = \frac{h}{m_e v_e} = 1.2\times10^{-10}\,m$$

Classical radius: e^- can be viewed as a particle with radius r_e:

$$r_e = \frac{e^2}{m_e c^2} = 2.82\times10^{-13}\,cm$$

Compton Wavelength:
Distance at which quantum effects cannot be ignored

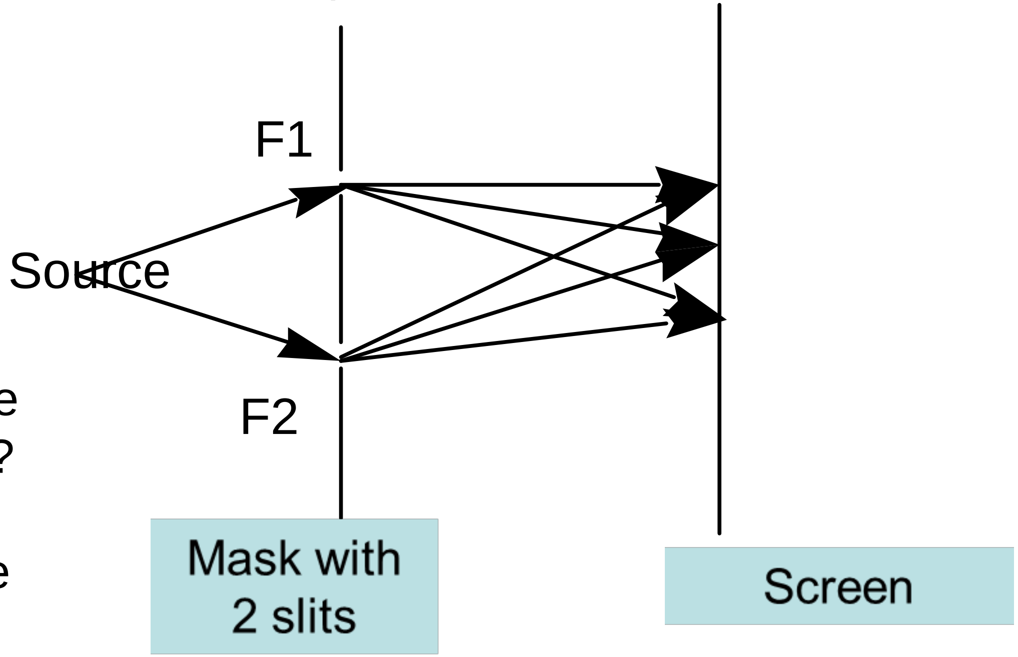
$$\lambda_c = \frac{h}{mc} = 2.43\times10^{-10}\,cm$$

Young's Double Slit Experiment

This is a typical experiment showing the wave nature of light and interferences.

What happens when we decrease the light intensity ?
If radiation = particles, individual photons reach one spot and there will be no interferences
If radiation $\neq$ particles there will be no spots on the screen

The result is ambiguous
There are spots
The superposition of all the impacts make interferences



Assuming a single electron each time
What means interference with itself ?
What is its trajectory?
If it goes through F1, it should ignore the presence of F2

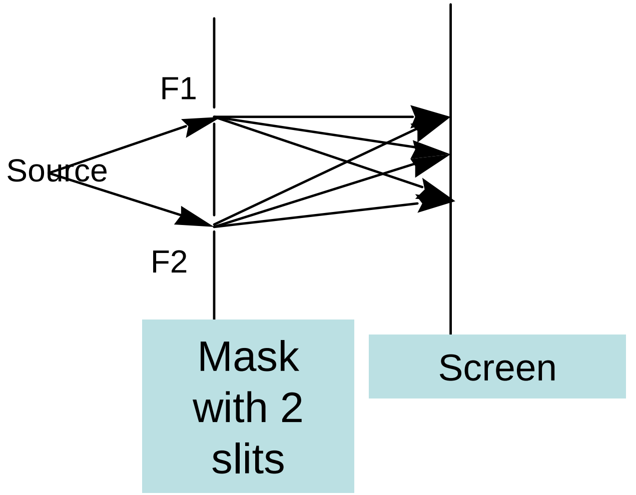
Young's Double Slit Experiment

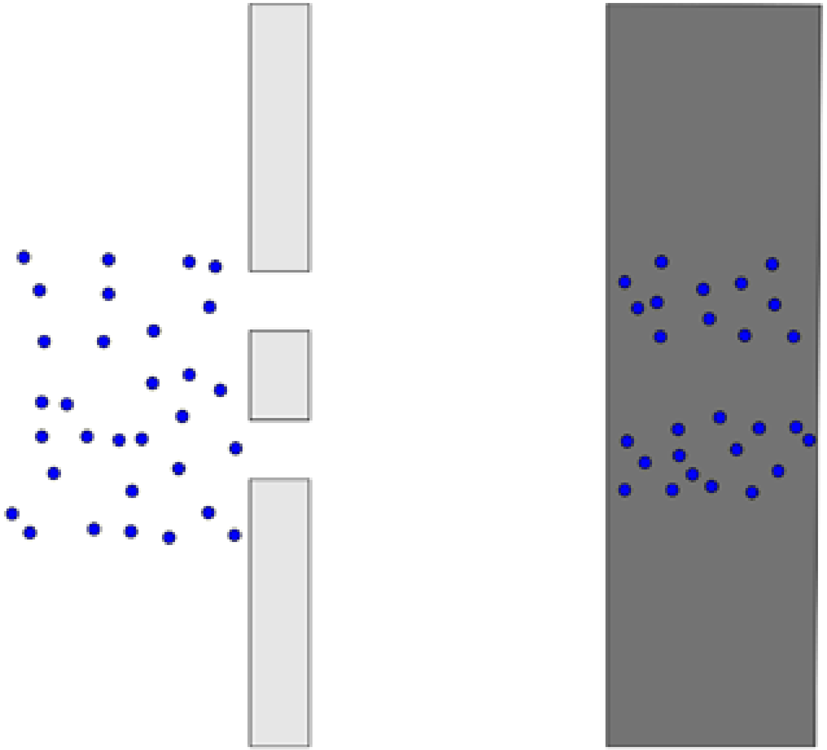
There is no possibility of knowing through which split the photon went!
If we measure the crossing through F1, we have to place a screen behind.
Then it does not go to the final screen.
We know that it goes through F1 but we do not know where it would go after.
These two questions are not compatible

Two important differences with classical physics:

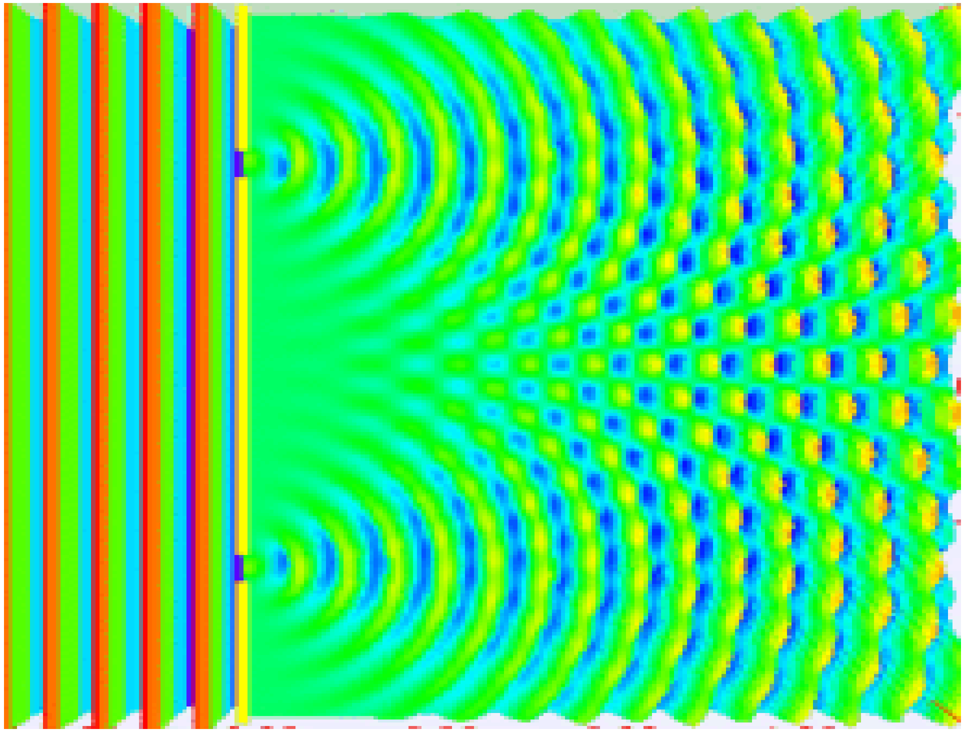
• measurement is not independent from observer

• trajectories are not defined; hν goes through F1 and F2 both! or through them with equal probabilities!

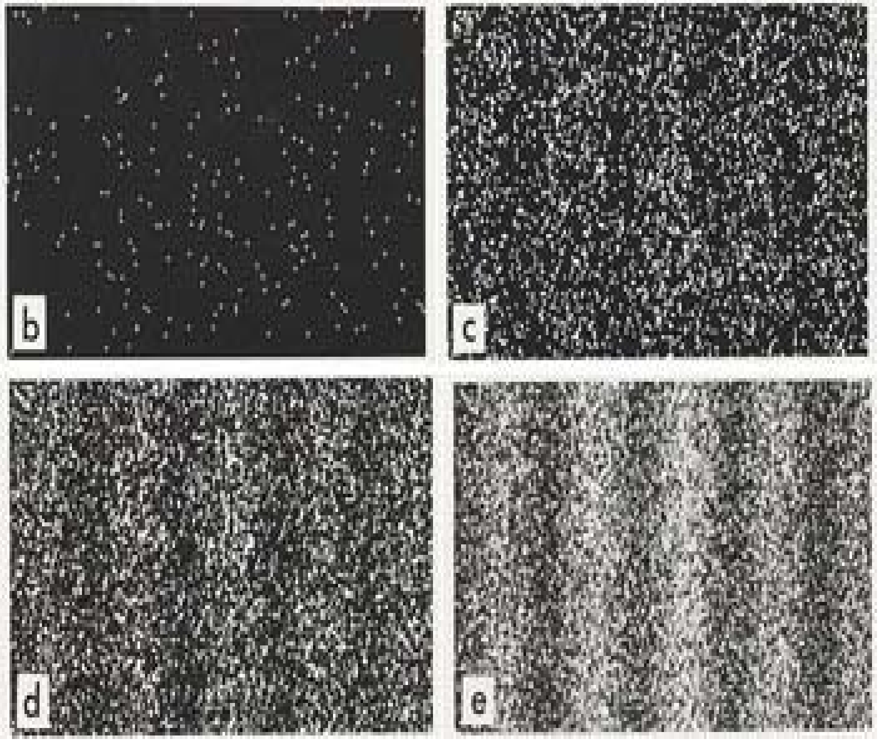




Optics: with light



QM: with electrons



Birth of Quantum Mechanics

- **The necessity for quantum mechanics was a series of observations.**
- **The theory of QM developed with a set of postulates.**
- **QM cannot be deduced from pure mathematical or logical reasoning.**
- **QM is not intuitive, because we cannot visualize atomic size.**
- **QM is based on observation. Like all science, it is subject to change if inconsistencies with further observation are revealed.**

New concepts in Quantum Mechanics:

Wave-Particle Duality

Superposition of states

Uncertainty Principle

Wave-Particle Duality

Wave interpretation of particles: Schrodinger formalism

- Wave functions

- Significance of wave function

- Normalisation

- The time-independent Schrödinger Equation.

- Solutions of the Schrödinger equation

The de Broglie Hypothesis

In 1924, de Broglie suggested that if waves of wavelength λ were associated with particles of momentum $p=h/\lambda$, then it should also work the other way round.

A particle of mass m, moving with velocity v has momentum p:

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

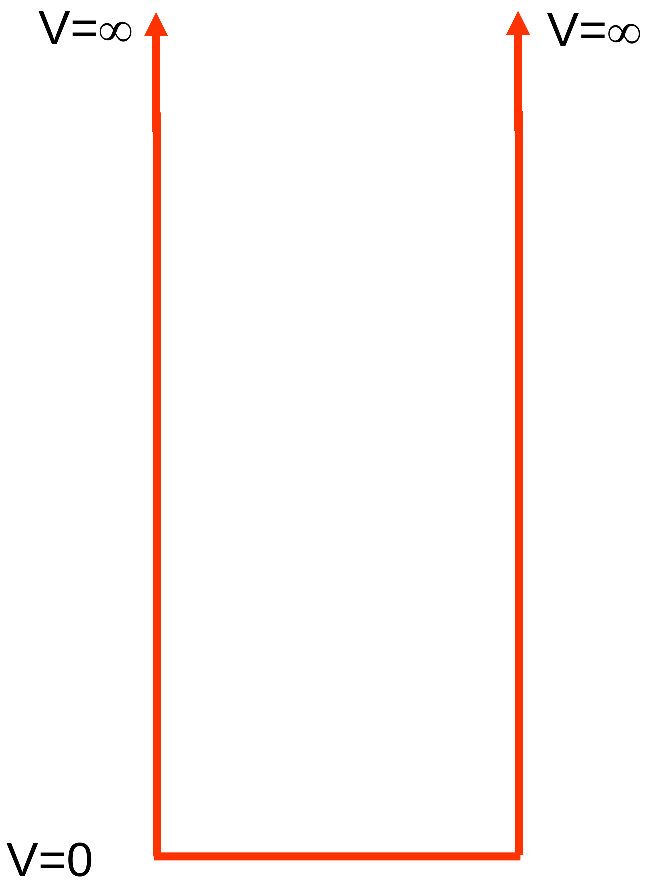
Kinetic Energy of particle

$$KE = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m}$$

$$\hbar = \frac{h}{2\pi}$$

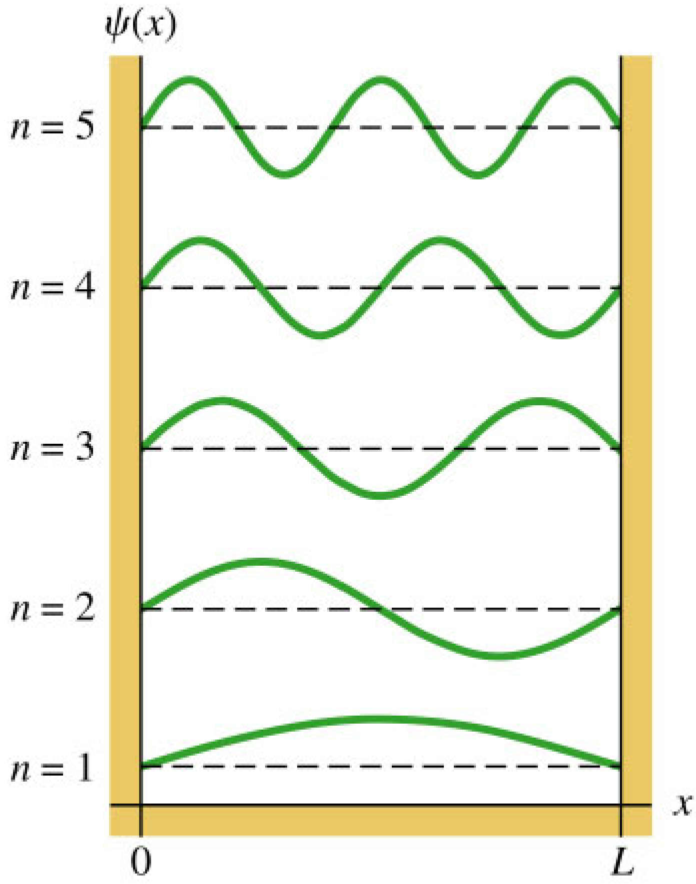
If the de Broglie hypothesis is correct, then a stream of classical particles should show evidence of wave-like characteristics.

Wavelengths of confined states



infinite potential well

In general, k =nπ/L, n= number of antinodes in standing wave



$$\lambda = \frac{2L}{3}\,;\, k = \frac{3\pi}{L}$$

$$\lambda = L\,;\, k = \frac{2\pi}{L}$$

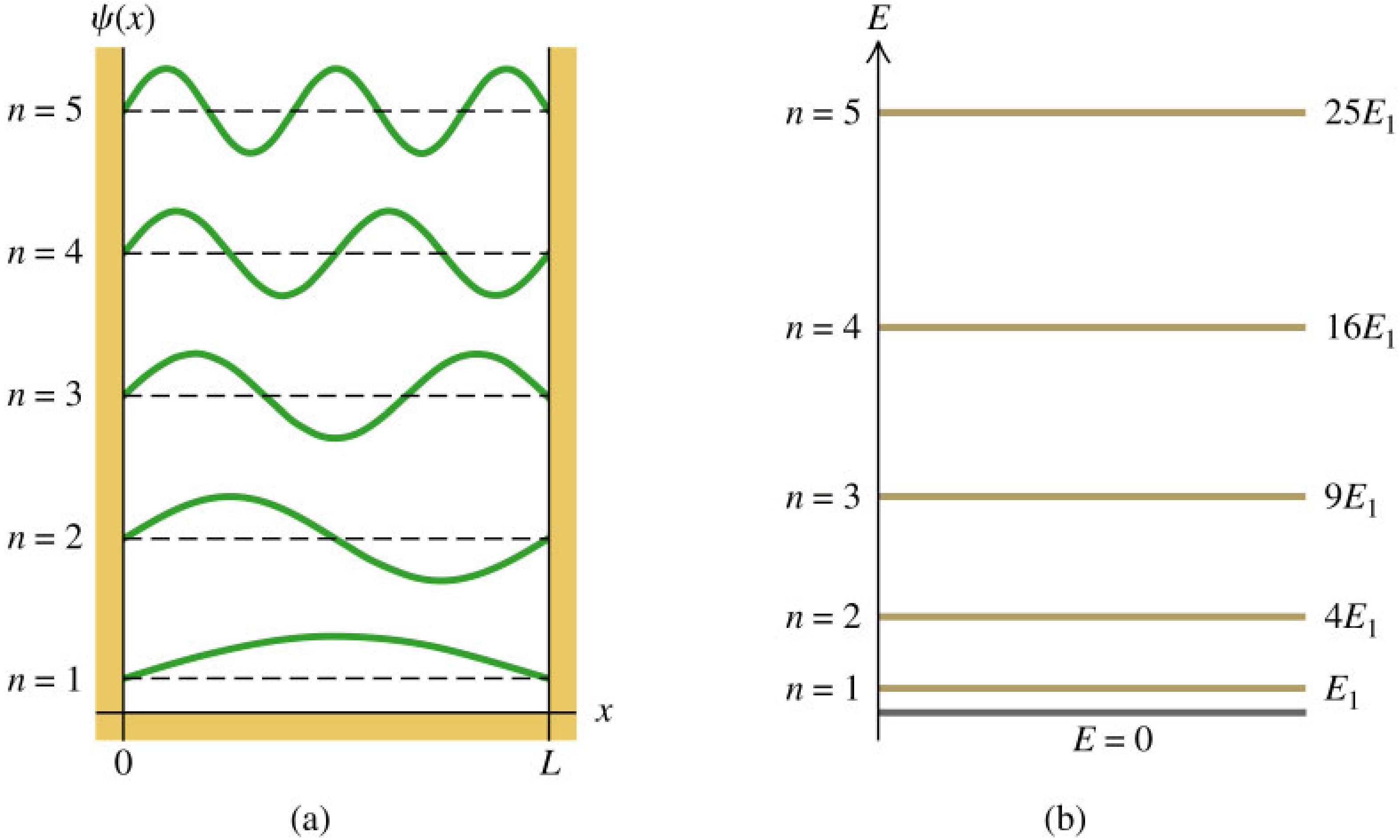
$$\lambda = 2L\,;\, k = \frac{\pi}{L}$$

Energies of confined states

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

$$E_n = n^2 E_1$$

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$$



Particle in a box: wave functions

Standing wave on a string has the form:

$$\boxed{y(x,t) = Ae^{i(\omega t - kx)} = A[(\cos\omega t + i\sin\omega t)(\cos kx - i\sin kx)]}$$

$$\text{Real part} = A[\cos\omega t\cos kx + \sin\omega t\sin kx]$$

Initial condition: y(0,t) = 0:

$$\boxed{y(x,t) = (A\sin kx)\sin(\omega t)}$$

Our particle in a box wave functions represent STATIONARY (time independent) states, so we write:

$$\boxed{\psi(x) = A\sin kx}$$

A is a constant, to be determined

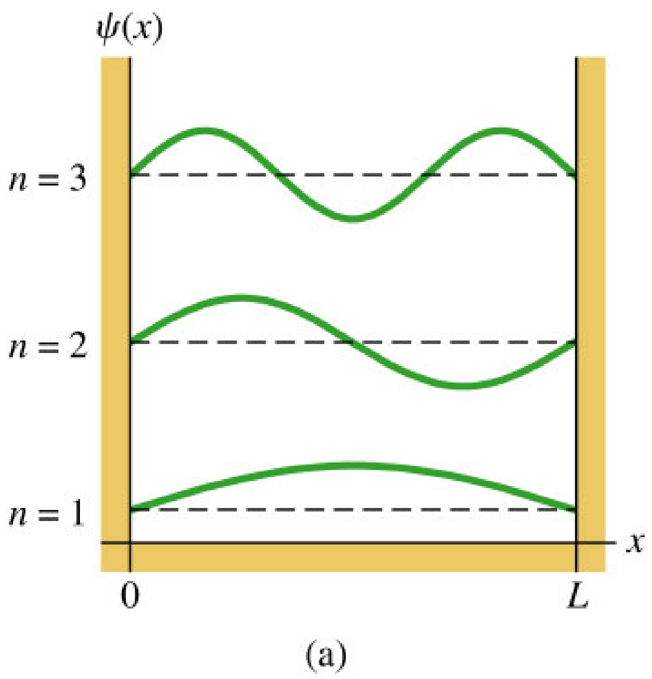
Interpretation of the wave function

The wave function of a particle is related to the *probability density.*

Probability of finding a particle between x and x + dx: $\left|\psi(x)\right|^2 dx$

The wave function is normalized by stating that the total probability of finding the particle somewhere = 1:

$$\int_{-\infty}^{+\infty} \left|\psi(x)\right|^2 dx = 1$$



Particle in a box: normalization of wave functions

Normalization condition determines one constant in the wave function. For our particle in a box we have:

$$\psi(x) = A\sin kx = A\sin\frac{n\pi x}{L}$$

Since, in this case the particle is confined by INFINITE potential barriers, we know particle must be located between x=0 and x=L →Normalisation condition reduces to :

$$\int_0^L |\psi(x)|^2 dx = 1$$

$$\Rightarrow \quad A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$\Rightarrow \quad \psi(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}$$

SCHRÖDINGER EQUATION

So far we have only treated a very simple one-dimensional case of a particle in a completely confining potential.

A general treatment of any problem requires the development of a more sophisticated "QUANTUM MECHANICS" based on the

SCHRÖDINGER EQUATION

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

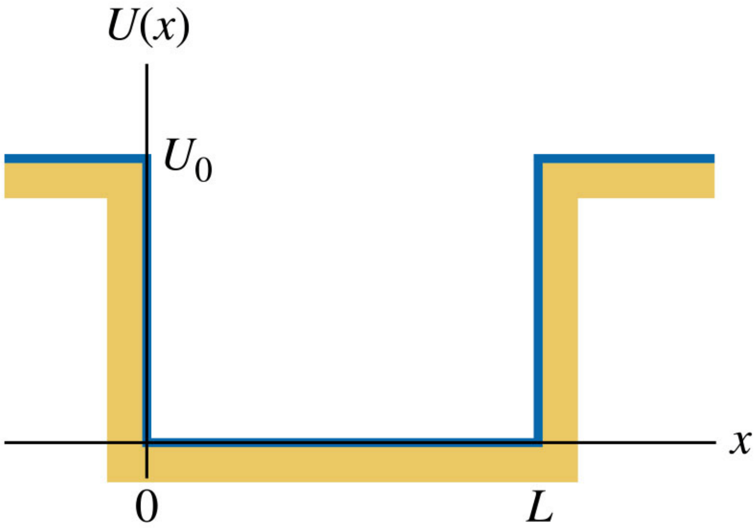
KE Term

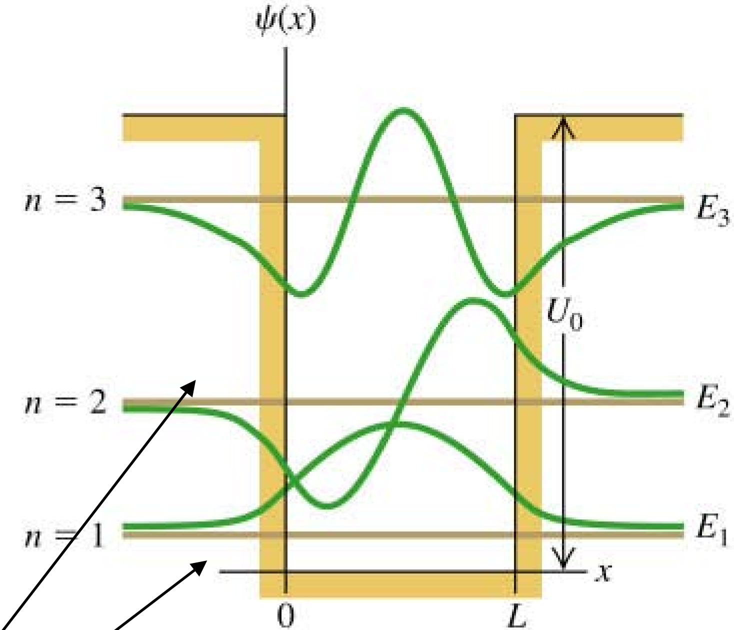
PE Term

In 1-dimension (time-independent)

Solving the Schrodinger equation allows us to calculate particle wave functions for a wide range of situations

Finite potential well



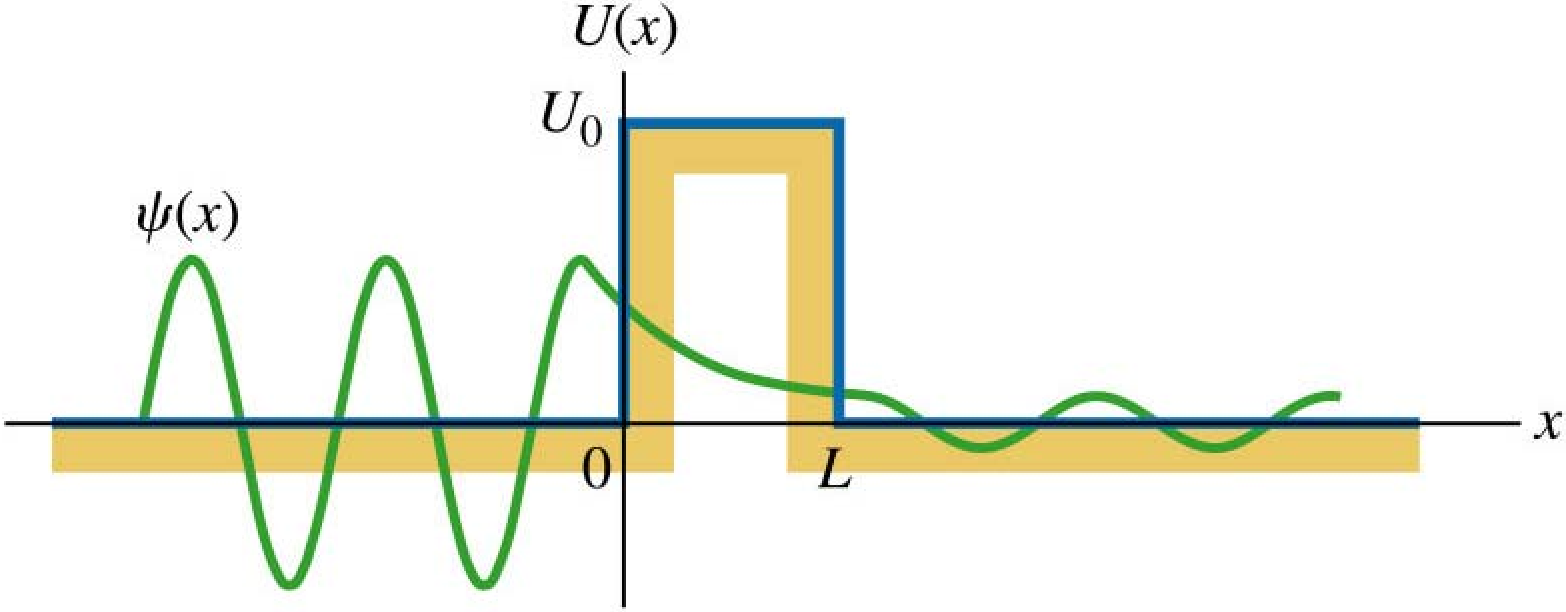


(a)

WF “leakage”, particle has finite probability of being found in barrier: CLASSICALLY FORBIDDEN

Solving the Schrodinger equation allows us to calculate particle wave functions for a wide range of situations

Barrier Penetration (Tunnelling)



Quantum mechanics allows particles to travel through “brick walls”!!!!

Solving the Schrodinger equation for particle in an infinite potential well

$$V(x) = 0 \qquad\qquad 0 < \mathrm{x} < \mathrm{L}$$

So, for 0<x<L, the time independent SE reduces to:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE\psi(x)}{\hbar^2} = 0$$

General Solution:

$$\boxed{\psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{1/2} x + B\cos\left(\frac{2mE}{\hbar^2}\right)^{1/2} x}$$

Boundary condition: ψ(x) = 0 when x=0:→B=0

$$\psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{1/2} x$$

Boundary condition: ψ(x) = 0 when x=L:

$$\psi(0) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{1/2} L = 0 \quad \Rightarrow \quad E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$\psi(x) = A\sin\frac{n\pi x}{L}$$

In agreement with the "fitting waves in boxes" treatment earlier.

Fundamental postulates of QM

- How is the physical state described?
- How are physical observables represented?
- What are the results of measurement?
- How does the physical state evolve in time?

These postulates are fundamental, and cannot be explained by any theory.
The theory is rather concerned with the consequences of these postulates.

Superposition of States:

If two states |a> and |b> are equally probable to any system |S>, Quantum Mechanics would treat both the states on equal footing:

$$\left|S\right\rangle = \frac{1}{\sqrt{2}}\left(\left|a\right\rangle + \left|b\right\rangle\right)$$

Any observation would find the system in the state |a> or |b>
Probability of getting result a or b depends on relative weights of A and B in the superposition.

Act of observation of a small Q. M. system causes a non-negligible disturbance.

Therefore, the results of one observation will not allow a causal prediction of the results of a subsequent observation.

Indeterminacy comes in calculation of observables.
Act of observation destroys causality.
Theory gives probability of obtaining a particular result.

Linear Algebra of Quantum Mechanics

The mathematical structure QM describes is a linear algebra of operators acting on a vector space.

Under Dirac notation, we denote a vector using a “ket”:

$$|v\rangle$$

The basic properties of vectors:

* $c|v\rangle$ is another vector

* $|v\rangle + |w\rangle$ is another vector

* null vector: $|v\rangle - |v\rangle = 0$

$$0|v\rangle = 0$$

A set of vectors $|1\rangle,\ |2\rangle,\ \ldots,\ |n\rangle$ are linear independent if
$c_1|1\rangle + c_2|2\rangle + \ldots + c_n|n\rangle = 0$ implies $c_1 = c_2 = \ldots = c_n = 0$.

A vector space is n-demensional if
the maximum number of linearly independent vectors in the space is n.

A set of n linearly independent vectors in n-dimensional space is a basis
--- any vector can be written in a unique way as a sum over a basis:

$$|v\rangle = \sum_{i=1}^{n} v_i |i\rangle$$

Once the basis is chosen, a vector can be represented by a column vector:

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}$$

A ket vector $|v\rangle$ is associated with a bra vector $\langle v|$ in the dual space.

The inner product of two ket vectors $|v\rangle$ and $|w\rangle$ are $\langle w|v\rangle = \langle v|w\rangle^*$

The dual of $c|v\rangle$ is $\langle v|c^*$.

The norm of $|v\rangle$ is defined as $|v| \equiv \sqrt{\langle v|v\rangle}$.

The Schwartz Inequality: $|\langle w|v\rangle|^2 \le |v|^2 |w|^2$.

Usually we require the basis to be orthonormal: $\langle i|j\rangle = \delta_{ij}$

A linearly independent set of basis vectors can be made orthonormal using the Gram-Schmidt procedure.

Give an orthonormal basis $\{|i\rangle\}$, and $|v\rangle = \sum v_i |i\rangle$,

$v_i = \langle i|v\rangle$

A linear operator $\hat{A}$ takes any vector in a linear vector space to another vector in that space: $\hat{A}|v\rangle = |v'\rangle$ and satisfies: $\hat{A}\left(c_1|v_1\rangle + c_2|v_2\rangle\right) = c_1|v_1'\rangle + c_2|v_2'\rangle$

Identity operator I : $I|v\rangle = |v\rangle$ for all $|v\rangle$.

For a n-dimensional space with an orthonormal basis $|1\rangle,\ |2\rangle,\ ...,\ |n\rangle$, the linear operator is completely determined by its action on the basis vectors, and the identity operator can be express as:

$$I = \sum_{i=1}^{n} |i\rangle\langle i|$$

Give an orthonormal basis $\{|i\rangle\}$, if $\hat{A}|v\rangle = |v'\rangle$, then $v_i' = A_{ij} v_j$

where $v_i' = \langle i | v' \rangle$, $v_i = \langle i | v \rangle$, $A_{ij} = \langle i | \hat{A} | j \rangle$

Therefore the action of $\hat{A}$ is simply equivalent to matrix multiplication:

$$\begin{pmatrix} v_1' \\ v_2' \\ \vdots \\ v_n' \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}$$

and $\hat{A}$ can then be represented by an $n \times n$ matrix.

If $\hat{A}\left|v\right\rangle = \left|v'\right\rangle$, then $\left\langle v'\right| = \left\langle v\right|\hat{A}^{\dagger}$. $\hat{A}^{\dagger}$ is called the adjoint of $\hat{A}$.

Give an orthonormal basis $\left\{\left|i\right\rangle\right\}$, like $\hat{A}$, $\hat{A}^{\dagger}$ can also be represented by an $n \times n$ matrix and the matrix elements of $\hat{A}$ and $\hat{A}^{\dagger}$ are related by

$$\left(A^{\dagger}\right)_{ij} = A^{*}_{ji}$$

An operator equal to its adjoint ($\hat{A} = \hat{A}^{\dagger}$), is called Hermitian.

An operator equal to minus its adjoint ($\hat{A} = -\hat{A}^{\dagger}$), is called anti-Hermitian.

An operator is unitary if $\hat{U}^{\dagger}\hat{U} = 1 = \hat{U}\hat{U}^{\dagger}$.

Unitary operator possesses the following properties:

It preserves the norm of a vector: if $|v'\rangle = \hat{U}|v\rangle$, then $|v'| = |v|$

It preserves the inner product: if $|v'\rangle = \hat{U}|v\rangle$ and $|w'\rangle = \hat{U}|w\rangle$, then $\langle v'|w'\rangle = \langle v|w\rangle$

It transforms one orthonormal basis in the space to another orthonormal basis.

Conversely, any transformation that takes one orthonormal basis to another must be unitary.

Eigenkets and Eigenvalues:

$$\hat{A}\left|a_i\right\rangle = a_i\left|a_i\right\rangle$$

Eigenvalues are roots to the characteristic polynomial

$$\det\left(A-\lambda I\right)=\begin{vmatrix} A_{11}-\lambda & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22}-\lambda & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn}-\lambda \end{vmatrix}$$

The set of eigenvalues of an operator satisfy:

$$\sum_{i=1}^{n} a_i = \sum_{i=1}^{n} A_{ii} = \mathrm{Tr}(A)$$

$$\prod_{i=1}^{n} a_i = \det(A)$$

Eigenkets and Eigenvalues of Hermitian Operators:

$$\hat{A}\left|a_i\right\rangle = a_i\left|a_i\right\rangle$$

All the eigenvalues are real.
Eigenkets belonging to different eigenvalues are orthogonal.
The complete eigenkets can form an orthonormal basis.
The operator can be written as $\hat{A} = \sum_{i=1}^{n} a_i \left|a_i\right\rangle\left\langle a_i\right|.$

Hermitian linear operator — **Real dynamical variable – represents observable quantity**

Eigenvector — **A state associated with an observable**

Eigenvalue — **Value of observable associated with a particular linear operator and eigenvector**

If $|a_i>$ are eigenvectors of A and $|b_i>$ are eigenvectors of B

$$A\left|a_i\right\rangle = a_i\left|a_i\right\rangle \qquad B\left|b_i\right\rangle = b_i\left|b_i\right\rangle$$

$$\left|b_i\right\rangle = \sum_i d_i\left|a_i\right\rangle \qquad \left|a_i\right\rangle = \sum_i f_i\left|b_i\right\rangle$$

$$\mathrm{A}\left|b_i\right\rangle = A\sum_i d_i\left|a_i\right\rangle = \sum_i d_i a_i\left|a_i\right\rangle$$

Measurement of an observable, which is represented by the operator A will find the system in one of the states $|a_i>$ with value a_i

Measurement of observable B will find the system in a combination of states $|b_i>$

Commuting operators:

[A,B] = AB-BA=0

A and B operators can have simultaneous eigenvalues.

$$\text{Let } |\alpha,\beta\rangle \text{ be the simultaneous eigenvalues of A and B}$$

$$\text{Then } \mathrm{A}|\alpha,\beta\rangle = \alpha|\alpha,\beta\rangle \quad \text{and} \quad \mathrm{B}|\alpha,\beta\rangle = \beta|\alpha,\beta\rangle$$

$$[\mathrm{A},\mathrm{B}]|\alpha,\beta\rangle = AB|\alpha,\beta\rangle - BA|\alpha,\beta\rangle = \alpha\beta|\alpha,\beta\rangle - \beta\alpha|\alpha,\beta\rangle = 0$$

Simultaneous measurements of A and B will find the system in one of the states $|\alpha,\beta\rangle$

Commutator and classical Poisson bracket $\{x,p_x\}$:

$$[x, p_x] = i\hbar\{x, p_x\} = i\hbar$$

$$\mathit{Classical} \quad \rightarrow \quad \text{Quantum}$$

$$\frac{dx}{dt} = \{x, H\} \rightarrow \frac{dx}{dt} = \frac{1}{i\hbar}[x, H]$$

$$\frac{dp}{dt} = \{p, H\} \rightarrow \frac{dp}{dt} = \frac{1}{i\hbar}[p, H]$$

Classical Mechanics

Newton

$$\vec{F} = m\frac{d^2\vec{x}}{dt^2}$$

$$\vec{F} = -G\frac{m_1 m_2}{|\vec{x}-\vec{x}'|^3}(\vec{x}-\vec{x}')$$

$$G = 6.6726 \times 10^{-11}\mathrm{m}^3 \cdot \mathrm{s}^{-2} \cdot \mathrm{kg}^{-1}$$

$$g = 9.8067\mathrm{m} \cdot \mathrm{s}^{-2}$$

Lagrangian

$$L = L(q, \dot{q}, t) = T - V$$

$$\delta S = 0$$

$$\frac{\partial L}{\partial q} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)$$

Hamiltonian

$$p = \frac{\partial L}{\partial \dot{q}}$$

$$H(q, p; t) = \sum_i p_i \dot{q}_i - L(q, \dot{q}; t)$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

Classical Mechanics

$$L = L(q, \dot{q}, t) = T - V$$

$$\boxed{p = \frac{\partial L}{\partial \dot{q}}}$$

Poisson Bracket

$$\{f, g\} = \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_j}$$

$$\{q_i, q_j\} = 0;\ \{q_i, q_j\} = 0;\ \{q_i, p_j\} = \delta_{ij};$$

$$\delta_{\mathrm{ij}} = 1 \quad \text{for i = j} \quad \text{and} \quad \delta_{ij} = 0 \quad \text{for i} \neq \text{j}$$

$$\boxed{H(q, p; t) = \sum_i p_i \dot{q}_i - L(q, \dot{q}; t)}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = \{q_i, H\}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = \{p_i, H\}$$

Equation of motion of any dynamical variable:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial f}{\partial p_i}\frac{dp_i}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i}$$

$$= \frac{\partial f}{\partial t} + \{f, H\}$$

When $[A,B] \neq 0$

Simultaneous precise measurement of A and B is not possible

$$\textit{Define}\ \ \Delta A = A - \langle A \rangle$$

$$\langle A \rangle = \langle \alpha | A | \alpha \rangle \quad \text{is the expectation value of A in the state } |\alpha\rangle$$

$$[\Delta A, \Delta B] = [A, B]$$

$[A,B]^{+} = -[A,B]$ Anti-Hermitian with Imaginary eigenvalue

$\{A,B\}^{+} = \{AB+BA\}^{+} = \{A,B\}$ Hermitian with Real eigenvalue

$$\Delta A \Delta B = \frac{1}{2}[\Delta A, \Delta B] + \frac{1}{2}\{\Delta A, \Delta B\} = \frac{1}{2}[A,B] + \frac{1}{2}\{\Delta A, \Delta B\}$$

$$\left|\langle \Delta A \Delta B \rangle\right|^2 = \left|\frac{1}{2}[A,B]\right|^2 + \text{Real positive number}$$

$$\geq \frac{1}{4}\left|\langle [A,B] \rangle\right|^2$$

Using Schwarz inequality: $$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$$

$$\left\langle(\Delta A)^2\right\rangle\left\langle(\Delta B)^2\right\rangle \geq \left\langle(\Delta A)^2(\Delta B)^2\right\rangle \geq \frac{1}{4}\left|\langle[A,B]\rangle\right|^2$$

When A and B are cannonical variables, like, (x,p_x) or (t,E) satisfying commutation relations like

$$[x, p_x] = i\hbar\{x, p_x\} = i\hbar$$

$$where \quad \{x, p_x\} \quad \text{is the classical Poisson bracket}$$

satisfies the uncertainty principle

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

Uncertainty Principle

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$$

"There is a limit to the fineness of our powers of observation and the smallness of the accompanying disturbance, a limit which is inherent in the nature of things and can never be surpassed by improved technique or increased skill on the part of the observer."

Dirac

Position space wave function:

$$x\left|x_i\right\rangle = x_i\left|x_i\right\rangle \qquad \left\langle x_i \middle| x_j \right\rangle = \delta(x_i - x_j)$$

$$\text{Physical state} \qquad \left|\alpha\right\rangle = \int dx_i \left|x_i\right\rangle\left\langle x_i \middle| \alpha\right\rangle$$

$$\text{Wave function} \qquad \psi_\alpha(x_i) = \left\langle x_i \middle| \alpha \right\rangle$$

$$\left\langle \beta \middle| \alpha \right\rangle = \int dx_i \left\langle \beta \middle| x_i \right\rangle\left\langle x_i \middle| \alpha \right\rangle = \int dx_i \psi^*_\beta(x_i)\psi_\alpha(x_i)$$

$$\text{Expectation value:}$$

$$\left\langle \beta\right| X \left|\alpha\right\rangle = \left\langle \beta \middle| x_i \right\rangle\left\langle x_i \right| X \left| x_j \right\rangle\left\langle x_j \middle| \alpha \right\rangle = \int dx_i \int dx_j \psi^*_\beta(x_i) X \psi_\alpha(x_j)$$

Momentum space wave function:

Wave function $\varphi_\alpha(p_i) = \langle p_i | \alpha \rangle$

$$P|p_i\rangle = p_i|p_i\rangle \qquad \langle p_i | p_j \rangle = \delta(p_i - p_j)$$

Physical state $|\alpha\rangle = \int dp_i |p_i\rangle\langle p_i|\alpha\rangle$

Normalize: $\int dp_i \langle\alpha|p_i\rangle\langle p_i|\alpha\rangle = \int dp_i |\varphi_\alpha(p_i)|^2 = 1$

$$\psi_\alpha(x_i) = \left[\frac{1}{\sqrt{2\pi\hbar}}\right]\int dp_i \exp\left[\frac{ip_i x_i}{\hbar}\right]\varphi_\alpha(p_i)$$

$$\varphi_\alpha(p_i) = \left[\frac{1}{\sqrt{2\pi\hbar}}\right]\int dx_i \exp\left[-\frac{ip_i x_i}{\hbar}\right]\psi_\alpha(x_i)$$

Schrödinger Equation

$$H \rightarrow i\hbar \frac{\partial}{\partial t} \qquad P \rightarrow -i\hbar \frac{\partial}{\partial x} \qquad \mathrm{H}\left|\alpha_{\mathrm{n}}(t)\right\rangle = \mathrm{E}_{n}\left|\alpha_{\mathrm{n}}(t)\right\rangle = i\hbar \frac{\partial}{\partial t}\left|\alpha_{\mathrm{n}}(t)\right\rangle$$

$$\Rightarrow \left|\alpha_{\mathrm{n}}(t)\right\rangle = \left|\alpha_{\mathrm{n}}(0)\right\rangle \exp\left[-\frac{iE_n}{\hbar}t\right] \qquad \psi_n(x,t) = \psi_n(x,0)\exp\left[-\frac{iE_n}{\hbar}t\right]$$

$$H = T + V = \frac{p^2}{2m} + V$$

$$H\left|\alpha_n(t)\right\rangle = -\frac{p^2}{2m}\left|\alpha_n(t)\right\rangle + V\left|\alpha_n(t)\right\rangle$$

$$H\psi_n(x,t) = \frac{\hbar^2}{2m}\frac{\partial^2\psi_n(x,t)}{\partial x^2} + V(x)\psi_n(x,t)$$

$$= \mathrm{H}\psi_n(x,t) = i\hbar\frac{\partial\psi_n(x,t)}{\partial t} = E_n\psi_n(x,t)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n(x,t)}{\partial x^2} + V(x)\psi_n(x,t) = E_n\psi_n(x,t)$$