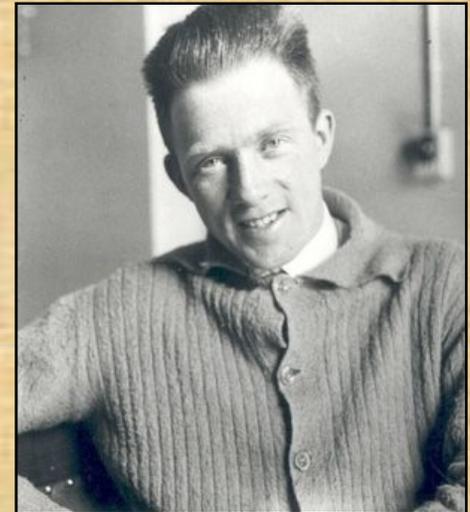
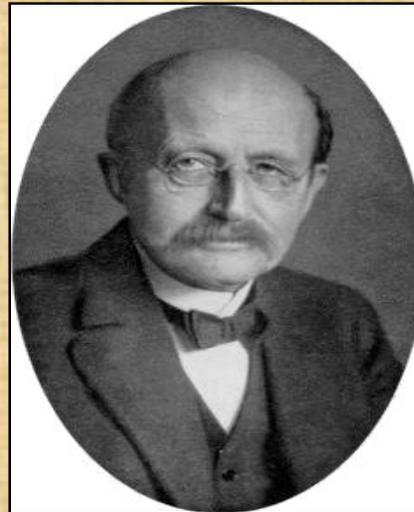
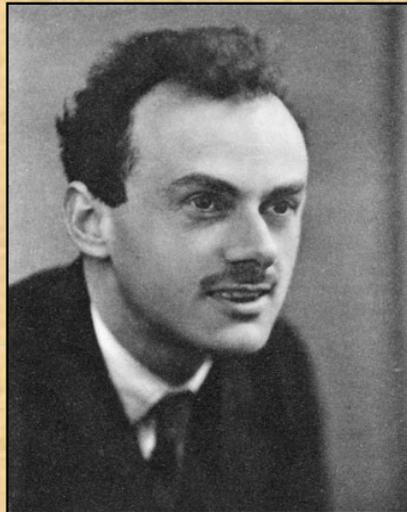


Quantization, Wave Function & Operators (Lesson 7)



Compiled by

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Associate Professor
Department of Chemistry
Surendranath College*

Topics of Interest:

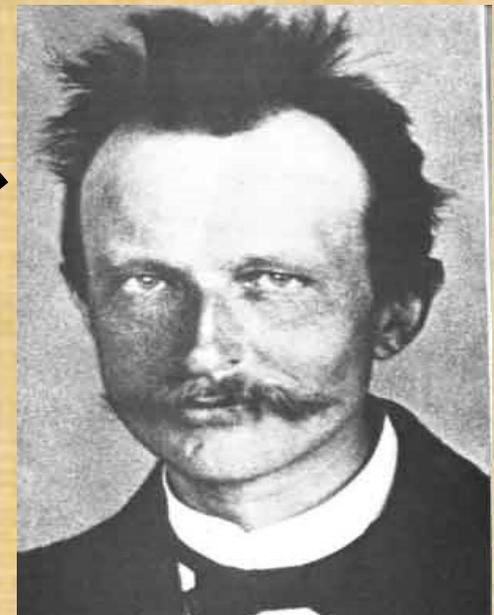
- *Quantisation, Wave Particle Duality*
- *Wave functions and operators*
- *Measurable physical quantities and associated operators - Correspondence principle*
- *The Schrödinger Equation*
- *The Uncertainty principle*

You already know h is the Planck constant in J.s

$$p = \hbar k = \frac{h}{\lambda} \quad ; \quad E = \hbar \omega = h\nu = \frac{h}{T} \quad \text{et} \quad v_{\phi} = \frac{E}{p}$$



Louis de BROGLIE
French
(1892-1987)



Max Planck (1901)
Göttingen

From Black-Body Radiation

Why a decrease for small λ ? Quantification!



**Max Planck
(1901)
Göttingen**



Numbering rungs of ladder introduces quantum numbers (here equally spaced)

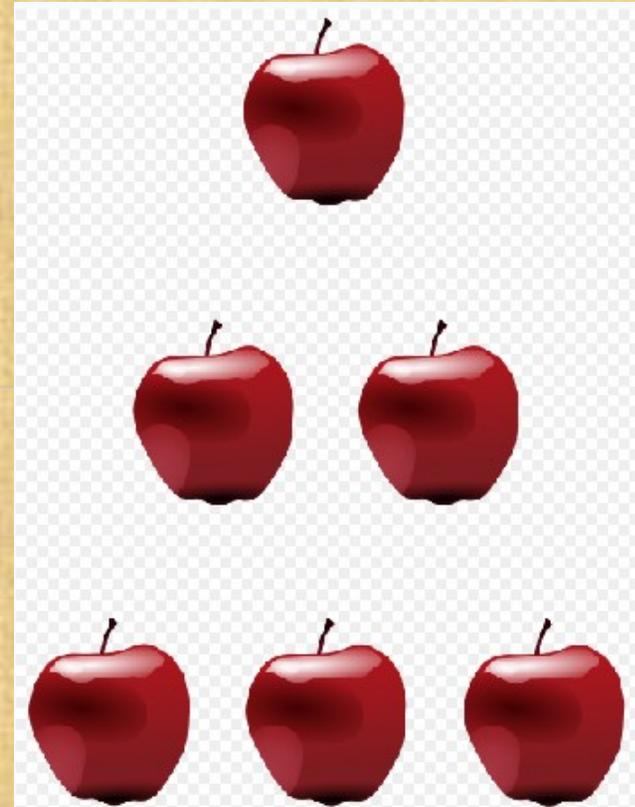


Quantum Numbers

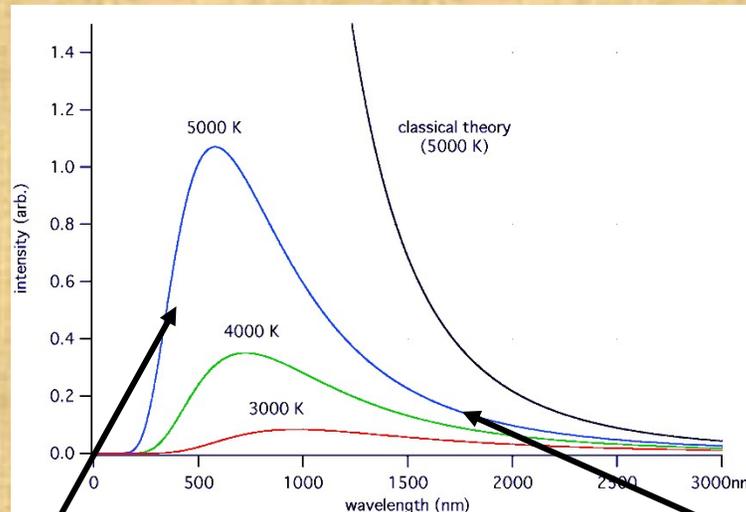
✓ In mathematics, a natural number (also called counting number) has two main purposes:

✓ they can be used for counting ("there are 6 apples on the table"), and also

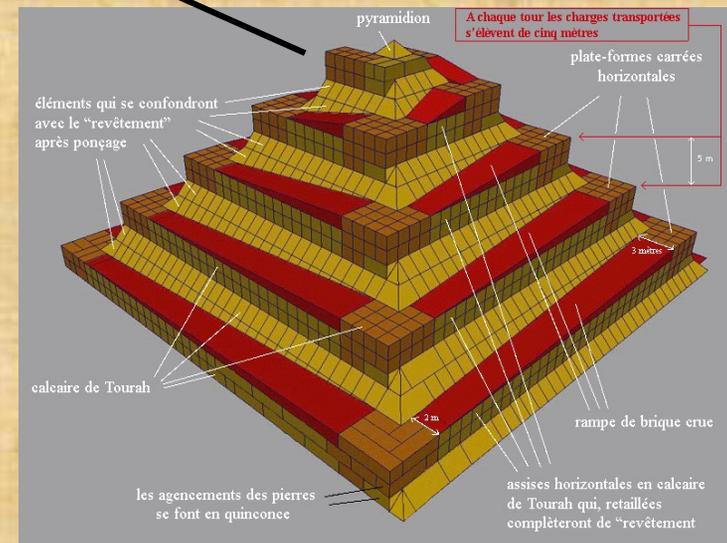
✓ they can be used for ordering ("this is the 3rd largest city in the country").



Black-Body Radiation, Quantification



**Steps too hard to climb
(Pyramid nowadays)**



**Easy slope, ramp
(Pyramid under construction)**

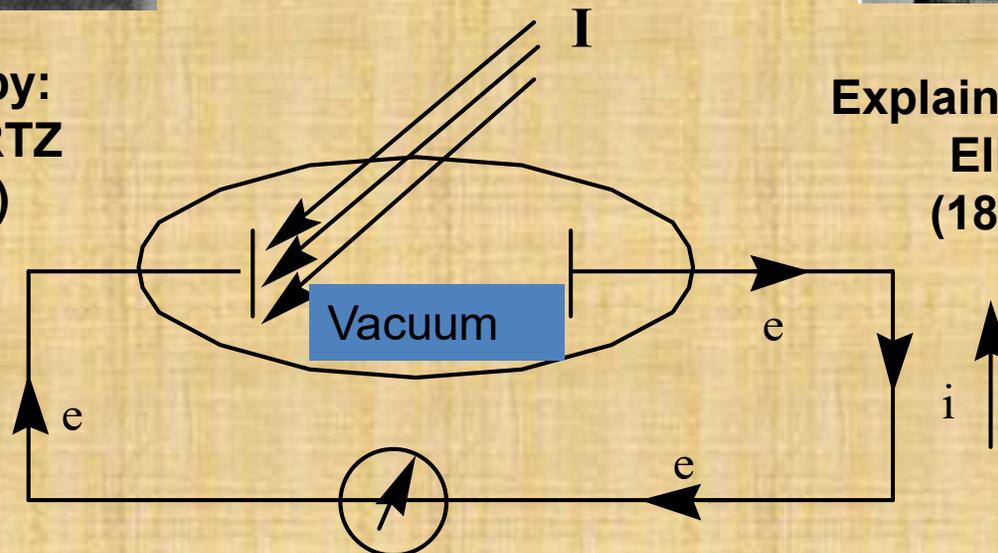


Photoelectric Effect (1887-1905)



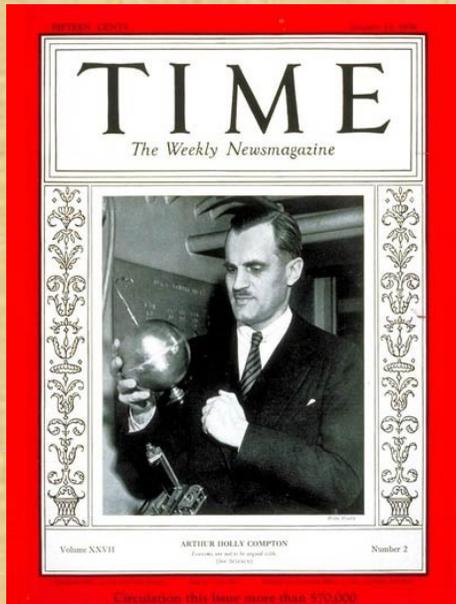
Discovered by:
Heinrich HERTZ
(1857-1894)

Explained by: **Albert EINSTEIN**
(1879-1955)

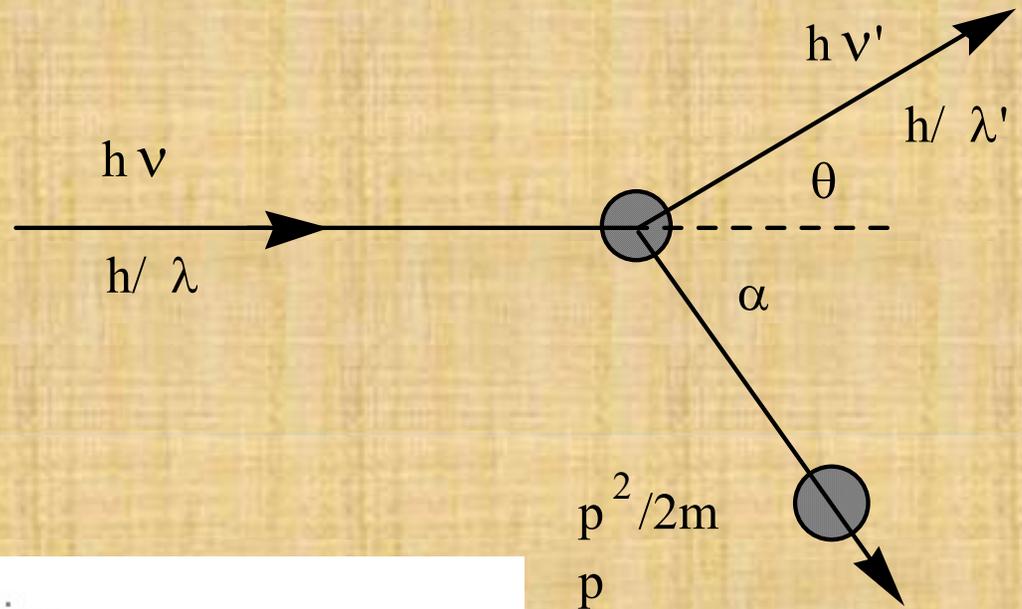


Compton Effect 1923

playing billiards assuming $l=h/p$



**Arthur Holly
Compton
American
1892-1962**



Energy Conservation

$$\hbar \frac{c}{\lambda} = \hbar \frac{c}{\lambda'} + \frac{p^2}{2m} \quad \left(v = \frac{c}{\lambda} \right)$$

Momentum Conservation (projection on x)

$$\frac{\hbar}{\lambda} = \frac{\hbar}{\lambda'} \cos \theta + p \cos \alpha$$

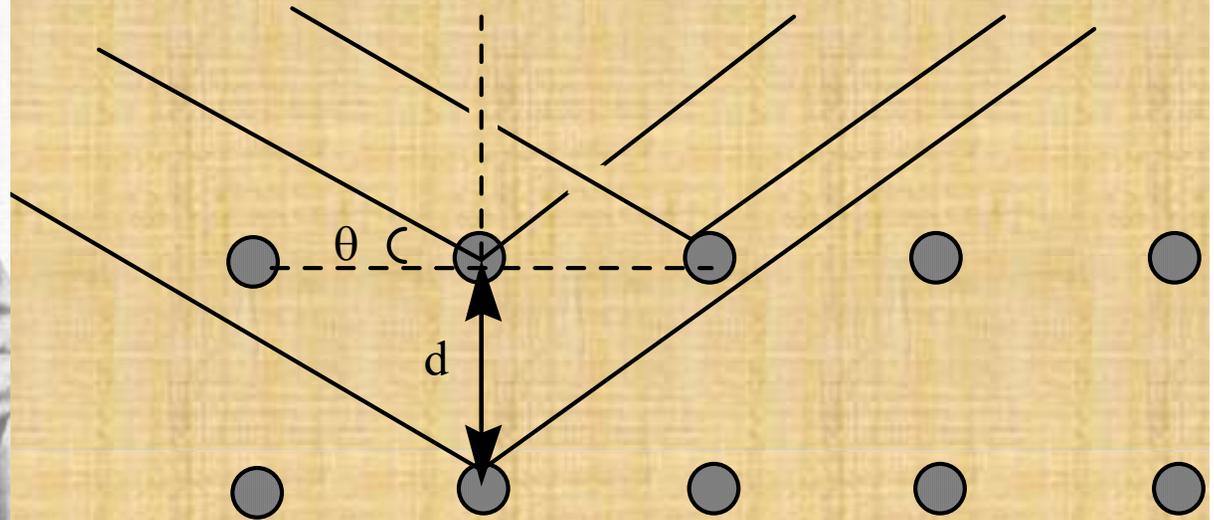
Momentum Conservation (projection on y)

$$0 = \frac{\hbar}{\lambda'} \sin \theta - p \sin \alpha$$

Davisson and Germer 1925



**Clinton Davisson
Lester Germer
In 1927**



$$2d \sin \theta = n \lambda$$

Diffraction is similarly observed using a mono-energetic electron beam

Bragg law is verified assuming $\lambda = h/p$

Wave–Particle Duality

In physics and chemistry, **wave–particle duality** is the concept that all matter and energy exhibits both wave-like and particle-like properties. A central concept of quantum mechanics, duality, addresses the inadequacy of classical concepts like "particle" and "wave" in fully describing the behavior of small-scale objects. Various interpretations of quantum mechanics attempt to explain this apparent paradox.

In Macroscopic World:

- A basket of cherries
- Many of them (identical)
- We can see them and taste others
- Taking one has negligible effect
- Cherries are both red and good



In Microscopic World:

- A single cherry
- Either we look at it without eating; It is red or, we eat it, it is good. (mutually exclusive)
- You can not try both at the same time. The cherry could not be good and red at the same time. (uncertainty & duality)





Slot machine “one-arm bandit”

After introducing a coin, you have 0 coin or X coins.

A measure of the profit has been made: profit = X

de Broglie Relation from Relativity

Popular expressions of relativity: m_0 is the mass at rest, m in motion



$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} \quad \text{and} \quad E = m c^2$$

E like to express $E(m)$ as $E(p)$ with $p=mv$

$$E^2 = m^2 c^4 \left(1 - \frac{v^2}{c^2}\right) + p^2 c^2 = m_0^2 c^4 + p^2 c^2$$

$$E = \sqrt{m_0^2 c^4 + p^2 c^2} = m_0 c^2 \left(1 + \frac{p^2}{m_0^2 c^2}\right)^{1/2} = E_i + \frac{p^2}{2m_0} + \dots$$

$$E_i + T + E_{\text{relativistic}} + \dots$$

de Broglie Relation from Relativity



$$E^2 = m_0^2 c^4 + p^2 c^2$$

Application to a photon ($m_0=0$)

$$E = h\nu$$

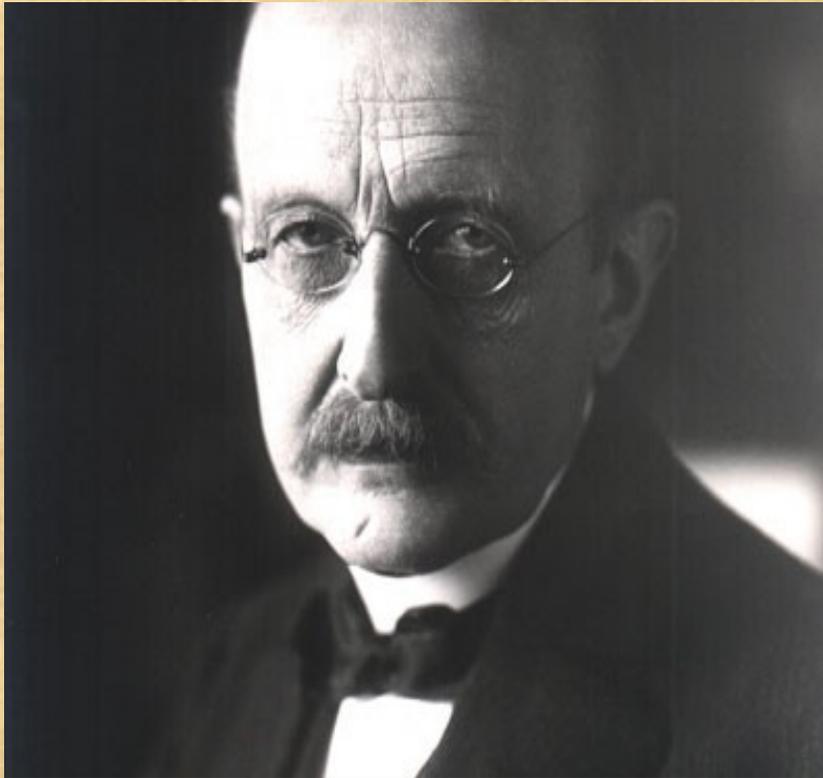
$$E = pc \rightarrow pc = h\nu$$

$$p = \frac{h\nu}{c} = \frac{h}{\lambda} = \frac{E}{c}$$

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

To remember

To remember



**Useful to remember to
relate energy and
wavelength**

Max Planck

$$\lambda = \frac{hc}{E} \rightarrow \lambda (\text{\AA}) = \frac{12410}{E(\text{eV})}$$

A New Mathematical Tool: Wave Functions & Operators

- ✓ Each particle may be described by a wave function $\Psi(x,y,z,t)$, real or complex, having a single value when position (x,y,z) and time (t) are defined.
- ✓ If it is not time-dependent, it is called stationary.
- ✓ The expression $\Psi=Ae^{i(pr-Et)}$ does not represent one molecule but a flow of particles: a plane wave

Wave Functions Describing One Particle

To represent a single particle $\Psi(x,y,z)$ that does not evolve in time, $\Psi(x,y,z)$ must be finite (0 at ∞).

In QM, a particle is not localized but has a probability to be in a given volume:

$dP = \Psi^* \Psi dV$ is the probability of finding the particle in the volume dV .
Around one point in space, the density of probability is $dP/dV = \Psi^* \Psi$

Ψ has the dimension of $L^{-1/3}$

Integration in the whole space should give one. That means Ψ is normalized.

$$\int_{total_space} \Psi^* \Psi dV = 1$$

Operators Associated to Physical Quantities

We cannot use functions (otherwise we would end with classical mechanics)

Any physical quantity is associated with an operator.

An **operator** \hat{O} is “the recipe to transform Y into Y' ”

We write: $\hat{O} Y = Y'$

If $\hat{O} Y = o Y$ (o is a number, meaning that \hat{O} does not modify Y , just a scaling factor), we say that Y is an **eigen function** of \hat{O} and o is the **eigen value**.

We have solved the **wave equation** $\hat{O} Y = o Y$ by finding simultaneously Y and o that satisfy the equation.

o is the **measure** of \hat{O} for the particle in the state described by Y .



O is a Vending machine (cans)

Introducing a coin, you get one can.

No measure of the gain is made unless you sell the can (return to coins)



Slot machine (one-arm bandit)

Introducing a coin, you have 0 coin or X coins.

A measure of the profit has been made: profit = X

Examples of Operators in Mathematics : Say P parity

$$Pf(x) = f(-x)$$

Even function : no change after $x \rightarrow -x$

Odd function : f changes sign after $x \rightarrow -x$

$y=x^2$ is even

$y=x^3$ is odd

$y= x^2 + x^3$ has no parity: $P(x^2 + x^3) = x^2 - x^3$

Examples of Operators in Mathematics: A

$$A = \frac{d^2}{dx^2} - x^2$$

Apply to the wave function $y = e^{-x^2/2}$

$$A y = \frac{d^2 y}{dx^2} - x^2 y = \frac{d^2 e^{-x^2/2}}{dx^2} + x^2 e^{-x^2/2}$$

$$A y = \frac{d(-x e^{-x^2/2})}{dx} - x^2 e^{-x^2/2} = -e^{-x^2/2} + x^2 e^{-x^2/2} - x^2 e^{-x^2/2}$$

$$A y = -e^{-x^2/2} = -y$$

Here, y is an eigen function; the eigen value is -1

Linearity

The operator \mathcal{O} is said to be linear:

$$\text{If } \mathcal{O}(aY_1 + bY_2) = \mathcal{O}(aY_1) + \mathcal{O}(bY_2)$$

Normalization

An eigen function remains an eigen function when multiplied by a constant.

That means, $\int \Psi^* \Psi dV = N$ thus it is always possible to normalize a finite function

$$\int_{total_space} \Psi^* \Psi dV = N \text{ taking } \Psi' = \frac{1}{\sqrt{N}} \Psi \text{ gives } \int_{total_space} \Psi'^* \Psi' dV = 1$$

Dirac notation is like: $\langle \Psi | \Psi \rangle$

Mean Value

• If Y_1 and Y_2 are associated with the same eigen value o : then,

$$O(aY_1 + bY_2) = o(aY_1 + bY_2)$$

• If not, then

$$• O(aY_1 + bY_2) = o_1(aY_1) + o_2(bY_2)$$

we define $\bar{o} = (a^2 o_1 + b^2 o_2) / (a^2 + b^2)$

$\Psi^* O \Psi = \Psi^* o \Psi$

o is a multiplying factor

$$\int_{-\infty}^{\infty} (\Psi^* O \Psi) dV = o \int_{-\infty}^{\infty} (\Psi^* \Psi) dV$$

$$o = \frac{\int_{-\infty}^{\infty} (\Psi^* O \Psi) dV}{\int_{-\infty}^{\infty} (\Psi^* \Psi) dV} = \frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Dirac notations

Sum, Product and Commutation of Operators

$$(A+B)\Psi = A\Psi + B\Psi$$

$$(AB)\Psi = A(B\Psi)$$

Eigen values

Wave functions

operators →

	$y_1 = e^{4x}$	$y_2 = x^2$	$y_3 = 1/x$
d/dx	4	--	--
x^3	3	3	3
$x \text{ d/dx}$	--	2	-1

Sum, Product and Commutation of Operators

$$[A,C] = AC - CA \neq 0$$

$$[A,B] = AB - BA = 0$$

$$[B,C] = BC - CB = 0$$

$$[A,C](y) = AC(y) - CA(y) = \frac{d}{dx} \left[x \frac{dy}{dx} \right] - x \left[\frac{d}{dx} \left(\frac{dy}{dx} \right) \right]$$

$$[A,C](y) = x \frac{d^2y}{dx^2} + \frac{dy}{dx} - x \frac{d^2y}{dx^2} = A(y)$$

$$[A,C] = A$$

	$y_1 = e^{4x}$	$y_2 = x^2$	$y_3 = 1/x$
$A = d/dx$	4	--	--
$B = x^3$	3	3	3
$C = x d/dx$	--	2	-1

non compatible operators

Compatibility, Incompatibility of Operators

$$[A,C]=AC-CA \neq 0$$

When the operators commute, the physical quantities may be simultaneously defined (compatibility)

$$[A,B]=AB-BA=0$$

$$[B,C]=BC-CB=0$$

When operators do not commute, the physical quantities can not be simultaneously defined (incompatibility). That means they are guided by the Heisenberg's Uncertainty Principle.

	$y_1=e^{4x}$	$y_2=x^2$	$y_3=1/x$
compatible operators $A = d/dx$	4	--	--
non compatible operators $B = x^3$	3	3	3
$C = x d/dx$	--	2	-1

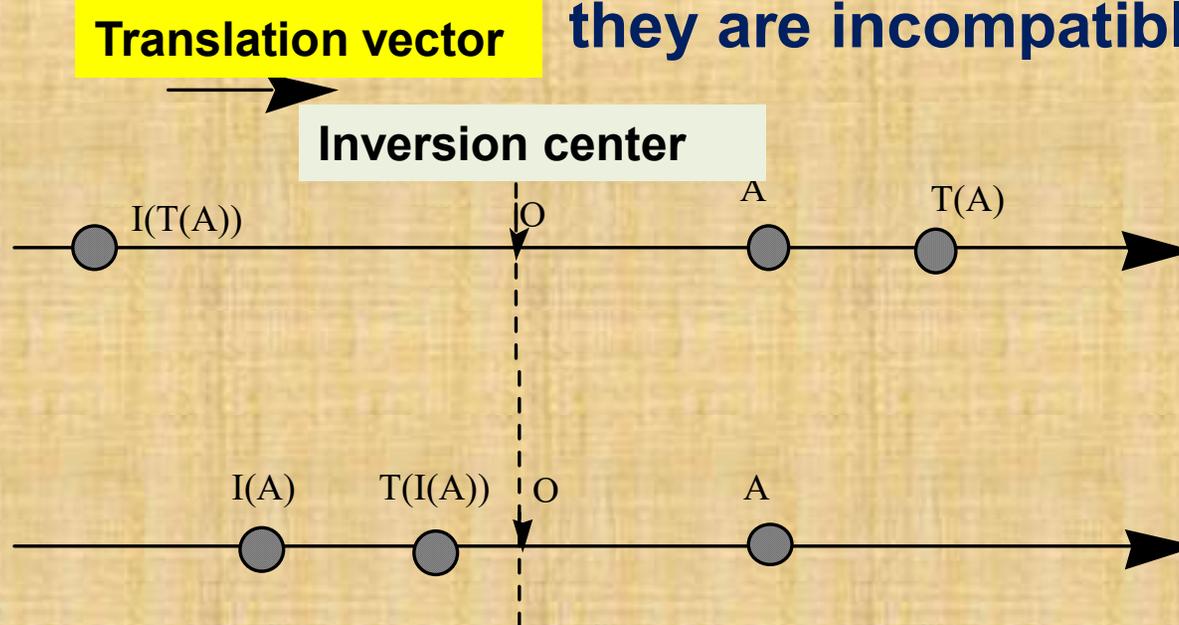
Look! x and d/dx do not commute, they are incompatible

$$[d/dx, x] = d/dx(x \cdot) - x(d/dx)$$

$$[d/dx, x](y) = \frac{d(xy)}{dx} - x \frac{dy}{dx} = x \frac{dy}{dx} + y - x \frac{dy}{dx} = y$$

$$[d/dx, x] = +1$$

Look! Translation and inversion also do not commute, they are incompatible too.....



Introducing New Variables!

Now it is time to give a physical meaning to the wave function. Where, p is the momentum, E is the Energy, $h=6.62 \cdot 10^{-34}$ J.s

$$p = \frac{h}{\lambda} \text{ and } E = h\nu$$

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

$$\Psi = A e^{i(kr - \omega t)} = A e^{2\pi i \left(\frac{r}{\lambda} - \nu t \right)} = A e^{\frac{i}{\hbar} (pr - Et)}$$

General Expression for Plane Waves

$$\Psi = A e^{i(kr - \omega t)} = A e^{2\pi i \left(\frac{r}{\lambda} - vt \right)} = A e^{\frac{i}{\hbar} (pr - Et)}$$

This represents a (monochromatic) beam, a continuous flow of particles with the same velocity (mono kinetic).

k , λ , ω , v , p and E are perfectly defined

R (position) and t (time) are not defined.

$\Psi\Psi^* = A^2 = \text{constant everywhere; there is no localization.}$

If $E = \text{constant}$, this is a stationary state, independent of t (time) which is not defined.

Correspondence Principle 1913/1920



Niels Henrik David Bohr

Danish
1885-1962

For every physical quantity one can define an **operator**. The definition uses formulae from classical physics replacing quantities involved by the corresponding operators.

QM is then built from classical physics in spite of demonstrating its limits.

Operators p and H

We would use expression of the plane wave stated earlier as it allows defining exactly both p and E .

Momentum and Energy Operators

$$\Psi(r,t) = \Psi(r) \Psi(t) = A e^{\frac{i}{\hbar}(pr)} e^{\frac{i}{\hbar}(-Et)}$$

$$\Psi(r) = A e^{\frac{i}{\hbar}(pr)} \quad \Psi(t) = e^{\frac{i}{\hbar}(-Et)}$$

$$\frac{\partial \Psi}{\partial r} = \frac{ip}{\hbar} \Psi \quad \text{and} \quad \frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar} \Psi$$

$$\text{therefore } \mathbf{p} = \frac{\hbar}{i} \frac{\partial}{\partial r} \quad \text{and} \quad \mathbf{E} = i\hbar \frac{\partial}{\partial t}$$

Remember this during this chapter

Stationary State $E = \text{constant}$

$$\Psi(t) = e^{\frac{i}{\hbar}(-Et)}$$

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = E\Psi(r,t) = E\Psi(r)\Psi(t)$$

Remember this for 3 slides after

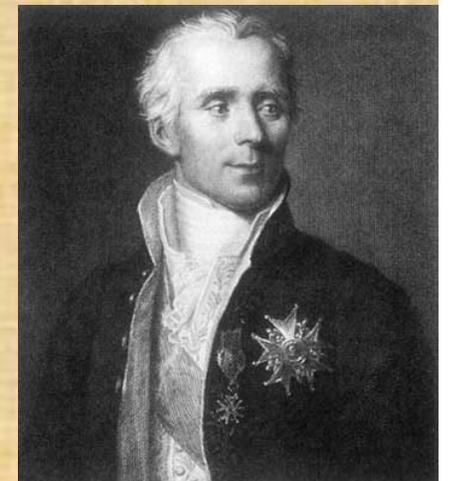
Kinetic Energy Operator

Classical $T = \frac{p^2}{2m}$ quantum operator $\hat{P}^2 = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$

In 3D : $T = \frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) = \frac{-\hbar^2}{2m} \Delta$

Calling $\Delta = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$ the Laplacian

*Pierre Simon,
Marquis de
Laplace
(1749 -1827)*



Correspondence Principle: Angular Momentum

Classical expression

$$L_z = xp_y - yp_x$$

Quantum expression

$$L_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

Quantum-mechanical Operators

Operator name	Symbol	Form	Notes
position (in x direction, for example)	\hat{x}	x	There are also corresponding operators for y, z.
position (three-dimensional, Cartesian coordinates)	$\hat{\mathbf{r}}$	$(x, y, z) = x\vec{x} + y\vec{y} + z\vec{z}$	
dipole moment (three-dimensional, Cartesian coordinates)	$\hat{\boldsymbol{\mu}}$	$\sum_{j=\text{all atoms}} q_j \mathbf{r}_j$	q is the charge on each atom; r is the position of each atom.
dipole moment (one atom in spherical coordinates)	$\hat{\boldsymbol{\mu}}$	$-e r (\vec{x} \sin \theta \cos \varphi + \vec{y} \sin \theta \sin \varphi + \vec{z} \cos \theta)$	
del	∇	$\vec{x} \frac{\partial}{\partial x} + \vec{y} \frac{\partial}{\partial y} + \vec{z} \frac{\partial}{\partial z}$	
Laplacian (three dimensional, Cartesian coordinates)	∇^2	$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$	
Laplacian (spherical coordinates)	∇^2	$\frac{1}{r^2} \left(\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right)$	
linear momentum (in x direction, for example)	\hat{p}_x	$-i \hbar \frac{\partial}{\partial x}$	There are also corresponding operators for y, z.

linear momentum (3 dimensions)	$\hat{\mathbf{p}}$	$-i\hbar\nabla$	
z-component of angular momentum	\hat{M}_z	$-i\hbar \frac{\partial}{\partial \varphi}$	
the square of total angular momentum	\hat{M}^2	$-\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right]$	
electronic angular momentum	$\hat{\mathbf{L}}$	$\hat{x} \hat{L}_x + \hat{y} \hat{L}_y + \hat{z} \hat{L}_z$	Operator has the same form as the angular momentum operator, \hat{M}
total energy (Hamiltonian)	\hat{H}	$\hat{T} + \hat{V}$	The potential energy (V) depends on the specific system being modeled. Additional energy terms can be added (e.g., interactions with electric or magnetic fields.)
kinetic energy for a single particle (Cartesian coordinates)	\hat{T}_x	$\left(\frac{-\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2}$	one-dimensional expression
	\hat{T}	$\left(\frac{-\hbar^2}{2m} \right) \nabla^2$	generalized expression
kinetic energy for a single particle (spherical coordinates)	\hat{T}	$\frac{-\hbar^2}{2\mu r^2} \left[\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right]$	

potential energy for a particle in a box	\hat{V}	$V = 0$ inside box $(0 \leq x \leq L)$ $V = \infty$ outside box $(x < 0, x > L)$	The box can be extended to 2 or 3 dimensions and the length of the box, L , can be different in each direction.
harmonic oscillator potential	\hat{V}	$\frac{K}{2} (x - x^e)^2$	For diatomic molecules; K is the force constant; x^e is the equilibrium bond length.
		$\frac{K}{2} \hat{Q}^2$	For polyatomic molecules; \hat{Q} is the operator for the magnitude of the normal coordinate.
Morse (anharmonic) potential	\hat{V}	$D_e (1 - e^{-\beta x})^2$	where x is the displacement of the oscillator from its equilibrium position, and D_e and β are constants or parameters.
Coulombic potential energy	\hat{V}	$\frac{q_1 q_2}{4\pi\epsilon_0 r_{12}}$	q is the charge on each particle; r is the distance between particles.
electric field	\hat{E}	E	Simple multiplicative operator as long as the field is constant over the area of interaction with the system.
magnetic field	\hat{B}	B	Operator is multiplicative and can be written without the caret.

magnetic moment of an electron	$\hat{\mu}_m$	$-\frac{e}{2m_e} \hat{L}$	
energy of interaction with a magnetic field	\hat{H}_m	$-\hat{\mu}_m \cdot \mathbf{B}$	general form
		$\frac{e}{2m_e} \hat{L} \cdot \mathbf{B}$	the particle is an electron and the magnetic field is directed along the z-axis
		$\frac{e B_z}{2m_e} \hat{L}_z$	
spin orbit interaction	\hat{H}_{s-o}	$\lambda \hat{S} \cdot \hat{L}$	
Coulomb operator	\hat{J}	$\hat{J}_j(1) \varphi_i(1) = \left[\int \varphi_i^*(2) \frac{1}{r_{12}} \varphi_i(2) d\tau_2 \right] \varphi_i(1)$	
Exchange operator	\hat{K}	$\hat{K}_j(1) \varphi_i(1) = \left[\int \varphi_j^*(2) \frac{1}{r_{12}} \varphi_i(2) d\tau_2 \right] \varphi_j(1)$	
Fock operator	\hat{F}	$\hat{H}^0 + \sum_{j=1}^N (2\hat{J}_j - \hat{K}_j)$	
		$-\frac{\hbar^2}{2m} \nabla^2 - \frac{Z e^2}{4\pi\epsilon_0 r} + \sum_{j=1}^N (2\hat{J}_j - \hat{K}_j)$	

Time-Dependent Schrödinger Equation



**Erwin Rudolf Josef Alexander
Schrödinger**
Austrian
1887 – 1961

Without potential $E = T$
With potential $E = T + V$

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

$$i\hbar \frac{\partial \Psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi(\mathbf{r},t) + V(\mathbf{r},t)\Psi(\mathbf{r},t)$$

Schrödinger Equation for stationary states

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi(\mathbf{r}, t) + V(\mathbf{r}, t) \Psi(\mathbf{r}, t)$$

$$\Psi(\mathbf{r}, t) = \Psi(\mathbf{r}) \cdot \Psi(t) = A \exp\left(\frac{-iEt}{\hbar}\right) \Psi(\mathbf{r})$$

$$i\hbar \frac{\partial \Psi(\mathbf{r}) \cdot \Psi(t)}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi(\mathbf{r}) \cdot \Psi(t) + V(\mathbf{r}) \Psi(\mathbf{r}) \cdot \Psi(t) = E \Psi(\mathbf{r}) \cdot \Psi(t)$$

$$-\frac{\hbar^2}{2m} \Delta \Psi(\mathbf{r}) + V(\mathbf{r}) \Psi(\mathbf{r}) = E \Psi(\mathbf{r})$$

Kinetic energy

Potential energy

Total energy

Schrödinger Equation for Stationary States

$$-\frac{\hbar^2}{2m} \Delta \Psi(\mathbf{r}) + V(\mathbf{r})\Psi(\mathbf{r}) = E \Psi(\mathbf{r})$$

$$\mathbb{H} \Psi(x,y,z) = E \Psi(x,y,z) \quad \text{with} \quad \mathbb{H} = -\frac{\hbar^2}{2m} \Delta + V$$

\mathbb{H} is the hamiltonian

Remember

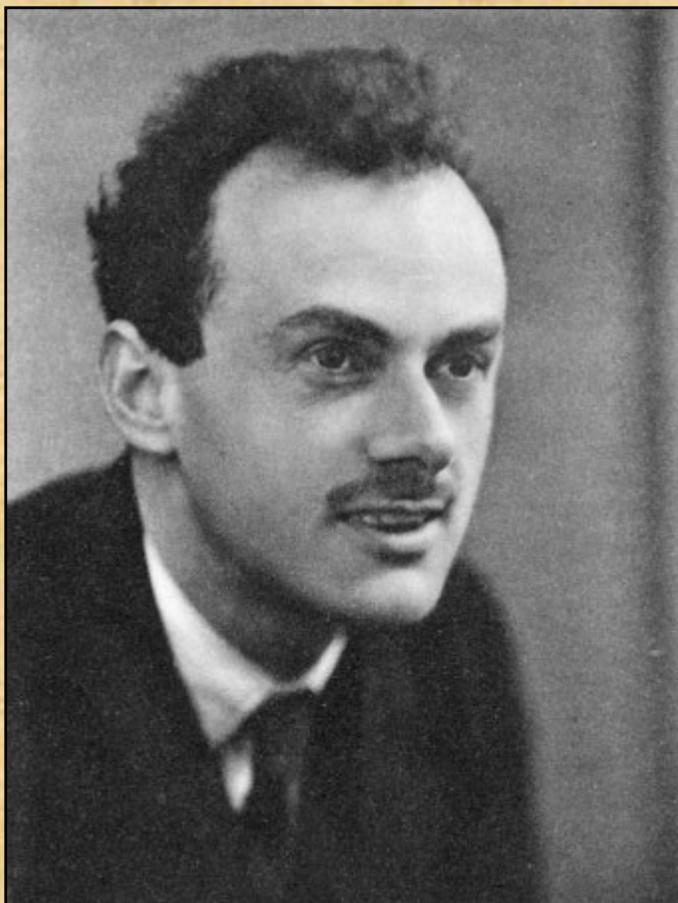


**Sir William Rowan
Hamilton**
Irish 1805-1865



Half penny bridge in Dublin

Chemistry is Nothing but an Application of Schrödinger Equation (Dirac)



Paul Adrien Dirac
1902 – 1984

$$\langle \Psi | \Psi \rangle \quad \langle \Psi | \color{red}{\mathbb{O}} | \Psi \rangle$$

Remember this Dirac notation, we would need later

Uncertainty Principle



Werner Heisenberg
German
1901-1976

The **Heisenberg uncertainty principle** states that locating a particle in a small region of space makes the momentum of the particle uncertain; and conversely, that measuring the momentum of a particle precisely makes the position uncertain. Remember, we already have seen incompatible operators!

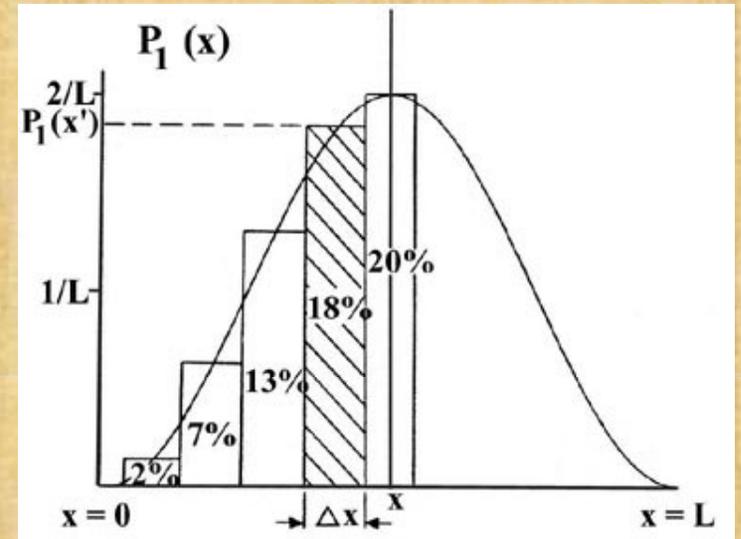
- It is not surprising to find that quantum mechanics does not predict the position of an electron exactly. Rather, it provides only a **probability** as to where the electron will be found.

- We shall illustrate the probability aspect in terms of the system of an electron confined to motion along a line of length L . Quantum mechanical probabilities are expressed in terms of a distribution function.

- For a plane wave, p is defined and the position is not.

- With a superposition of plane waves, we introduce an uncertainty on p and we localize. Since, the sum of 2 wave functions is neither an eigen function for p nor x , we have average values.

- With a Gaussian function, the localization below is $1/2p$



p and x do not commute and are hence incompatible.

For a plane wave, actually p is known and x is not, as $(Y^*Y=A^2)$ everywhere.

Let's superpose two waves...

$$\lambda_1 = \lambda + \frac{\Delta\lambda}{2} \text{ et } \lambda_2 = \lambda - \frac{\Delta\lambda}{2} .$$

this introduces a delocalization for p and may be localized x.

At the origin $x=0$ and at $t=0$, now if we want to increase the total amplitude, the two waves Y_1 and Y_2 are taken in phase. At $\pm Dx/2$ we want to impose them out of phase. The position is therefore known for $x \pm Dx/2$; the waves will have wavelengths.

$$\frac{x}{\lambda_1} - \frac{x}{\lambda_2} = \frac{1}{2} \quad \rightarrow \quad \frac{\frac{\Delta x}{2}}{\lambda + \frac{\Delta\lambda}{2}} - \frac{\frac{\Delta x}{2}}{\lambda - \frac{\Delta\lambda}{2}} = \frac{1}{2}$$

$$\frac{\frac{\Delta x}{2} (\lambda - \frac{\Delta\lambda}{2}) - \frac{\Delta x}{2} (\lambda + \frac{\Delta\lambda}{2})}{(\lambda + \frac{\Delta\lambda}{2})(\lambda - \frac{\Delta\lambda}{2})} = \frac{1}{2} = \frac{-\Delta x \Delta\lambda}{2\lambda^2}$$

$$\Delta x \Delta\lambda = -\lambda^2 \quad p = \frac{h}{\lambda} \rightarrow dp = \frac{-h d\lambda}{\lambda^2}$$

making $\Delta p = dp$ and $\Delta\lambda = d\lambda$

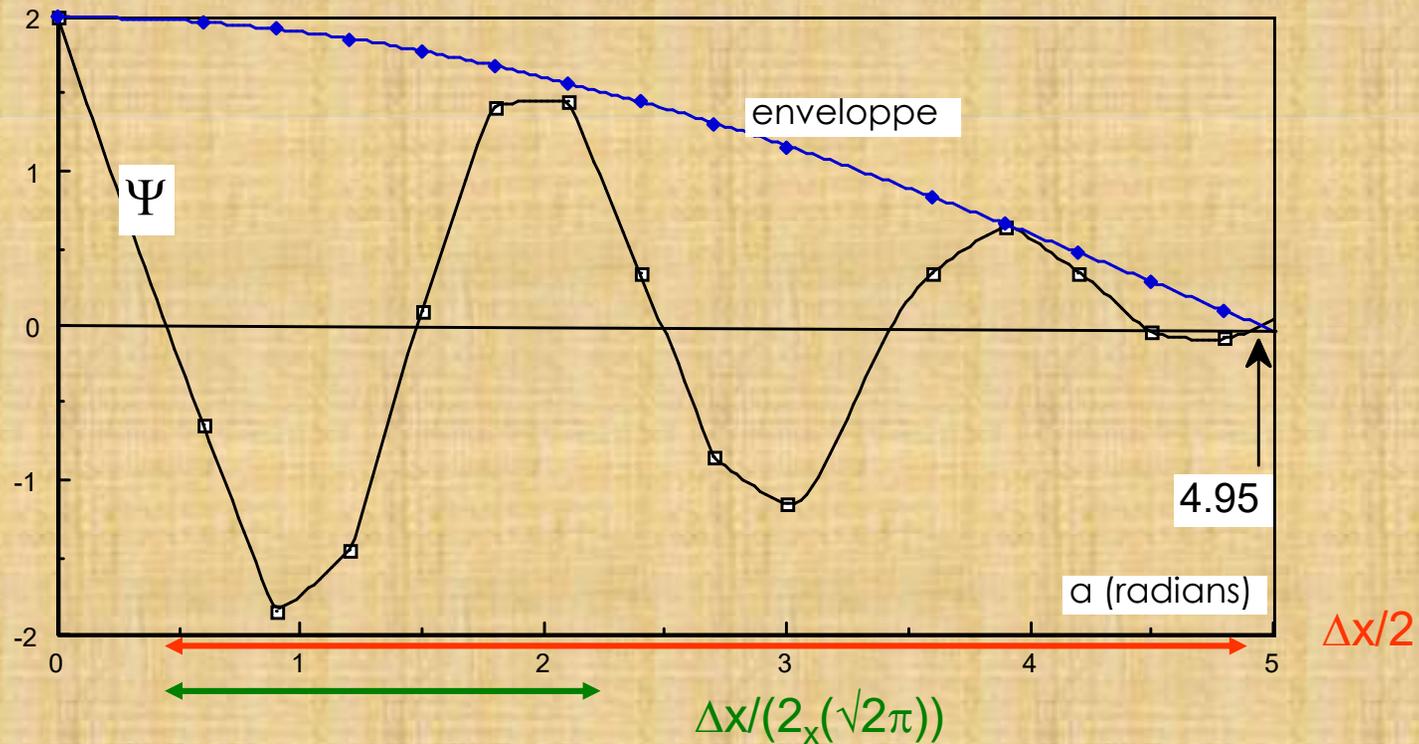
$$\rightarrow \quad \boxed{\Delta x \cdot \Delta p = h}$$

Superposition of Two Waves

$$\Psi = \cos(2\pi(\frac{x}{0.9} - vt)) + \cos(2\pi(\frac{x}{1.1} - vt)) = 2 \cos(\frac{\pi x}{9.9}) \cos(2\pi(\frac{x}{0.99} - vt))$$

$$\frac{\Delta x}{2} = 4.95 \quad \Delta \lambda = 1.1 - 0.9 = 0.2$$

$$\Delta x \cdot \Delta \lambda = 0.99 \text{ close to } \lambda^2 = 1$$



Uncertainty Principle



Werner Heisenberg
German
1901-1976

A more accurate calculation localizes the particles more and therefore one gets;

$$\Delta x \cdot \Delta p = \hbar$$

$$\Delta E \cdot \Delta t = \hbar$$

$$\hbar = 1.0536 \cdot 10^{-34} \text{ J}\cdot\text{s}$$

$$\Psi = A \exp\left(\frac{2\pi i}{h}(p x - E t)\right)$$

x and p or E and t play symmetric roles in the plane wave expression;

**Therefore, there are the two main
UNCERTAINTY PRINCIPLES**





Remember:

This much about
Functions and
Operators for now.
More on them in the
coming lessons!

THANK YOU!

THANK YOU!

ANY QUESTION?