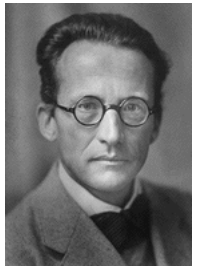
Lecture 11

End of Determinism
Rise of Probabilistic Mother Nature

$$\langle \mathcal{L} | \hat{\mathcal{A}} | \mathcal{R} \rangle$$

Consider Left and Right Slits !

Some happy unhappiness !



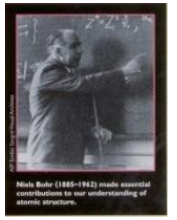
Schrodinger was not a fan of Heisenberg's matrix works !

"I naturally knew about his theory, but was discouraged, if not repelled, by what appeared to me as very difficult methods of transcendental algebra, and by the want of perspicuity."

$$QP - PQ = \frac{ih}{2\pi} = i\hbar$$

$$\Delta x \Delta p \approx \hbar$$

It was 1926, Schrodinger visited Bohr… exhausted by the discussions and fell ill but Bohr continued the dialogue at the bedside !



How can we comprehend all these ?

Hamilton draw parallels between :

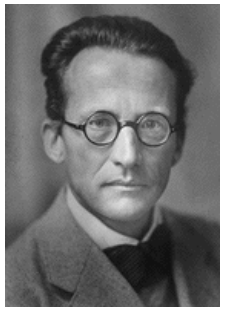
Optics and Mechanics

optics

$$\left[\nabla L(r)\right]^2 = n^2(r)$$

wave formula (Mechanics)

$$\left[\nabla W(r)\right]^2 = 2m\left[E - V\right]$$



$$\nabla^2\phi(r) = -\frac{4\pi^2}{\lambda^2}\phi(r)$$

Clue: Scalar optical wave equation

$$\frac{d^2\phi}{dx^2} + \frac{d^2\phi}{dy^2} + \frac{d^2\phi}{dz^2}$$

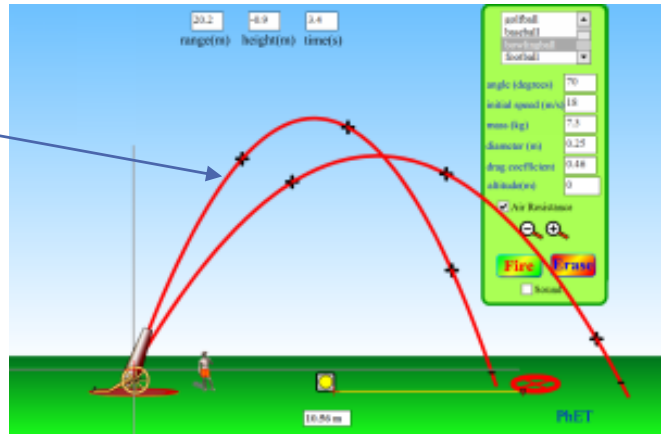
Schrodinger took inspiration from the above

$$\nabla^2\psi(r) = -\frac{8\pi^2 m}{h^2}\left(E - V\right)\psi(r)$$

The Famous Schrodinger Equation

Physics is where the Action is !

Consider projectile motion



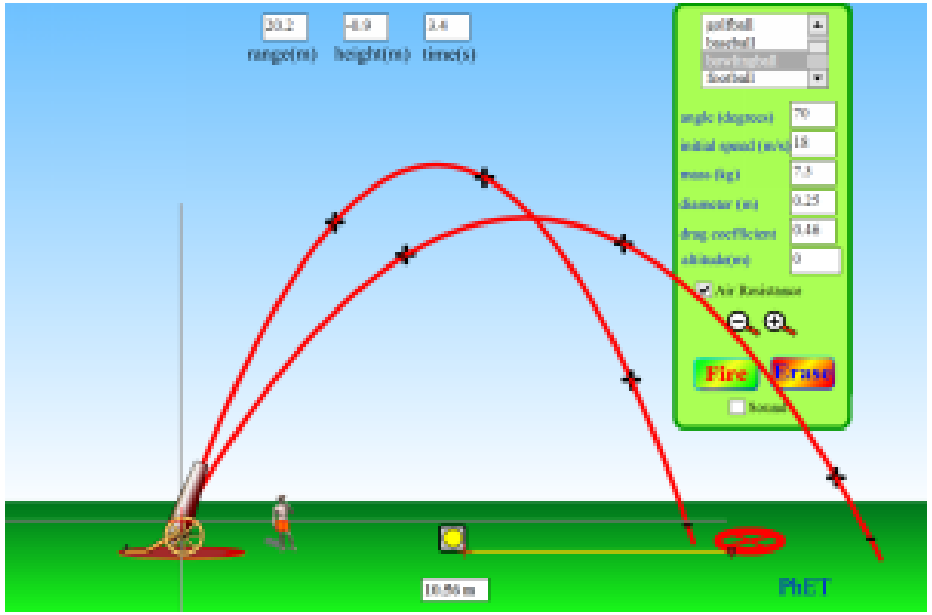
$$Action:\ S = \int_{t_1}^{t_2} (KE - PE)dt$$

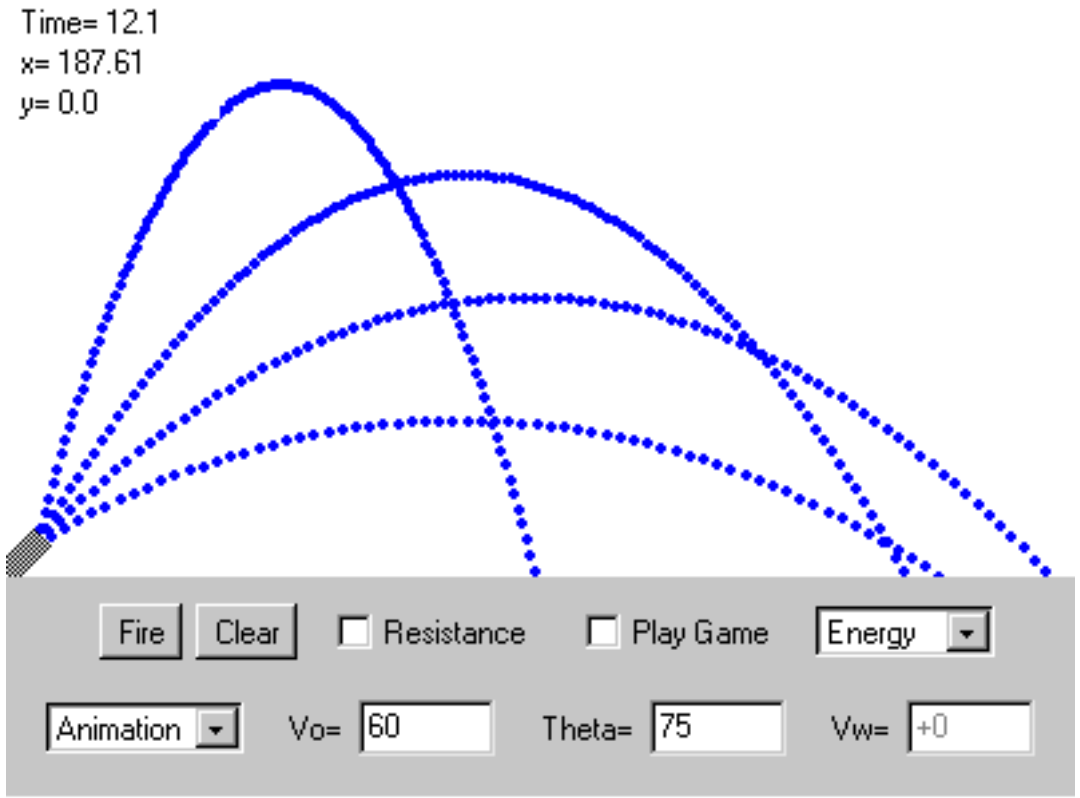
Of all the possible paths, the particle (light) would choose that for which the *"Action is the least"* … it is the path way to the equation of motion !

So how does a physicist study such a path ?

It just boils down to finding the successive states or how the states evolves with time. e.g. (*q, p*), *q* being the co-ordinate (position) and *p* the momentum.

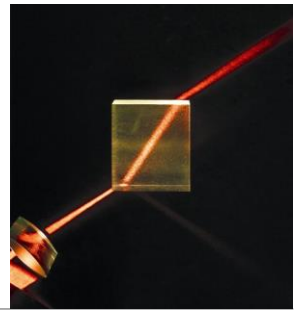
Consider Projectile Motion

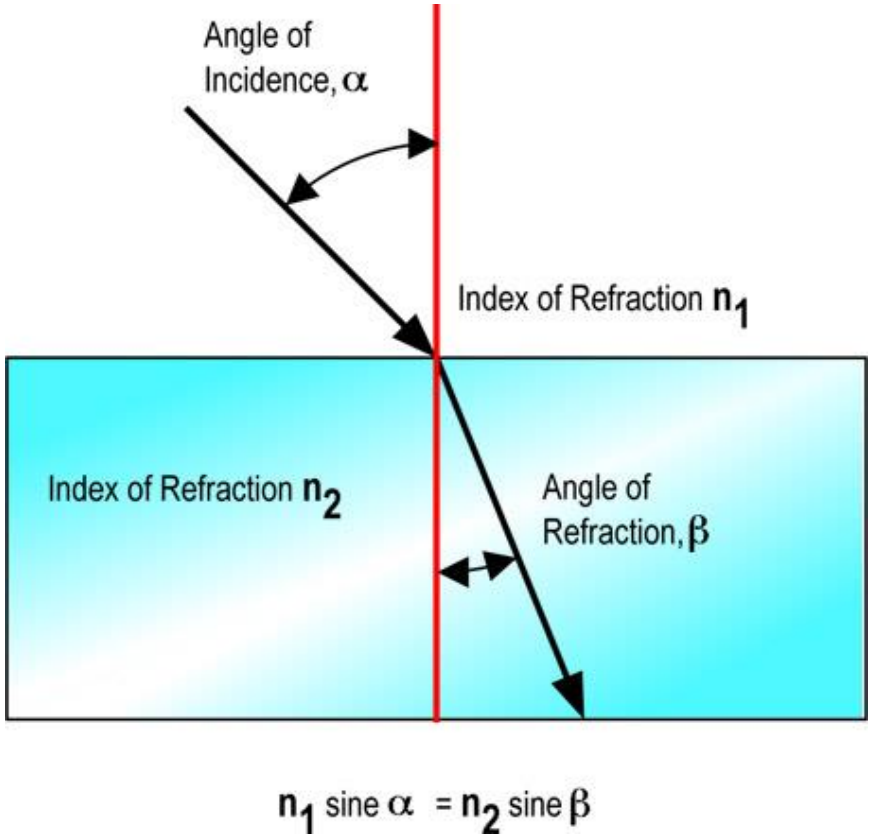




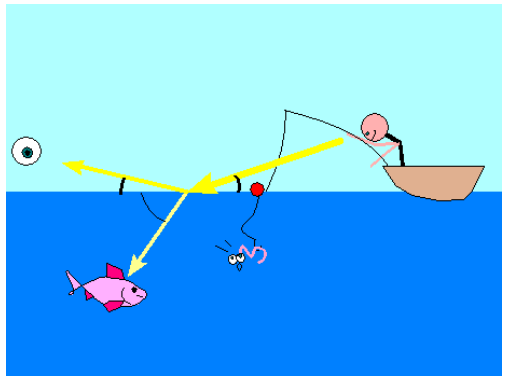
It just boils down to finding the successive states or how the states evolves with time. e.g. (q, p), q being the co-ordinate (position) and p the momentum.

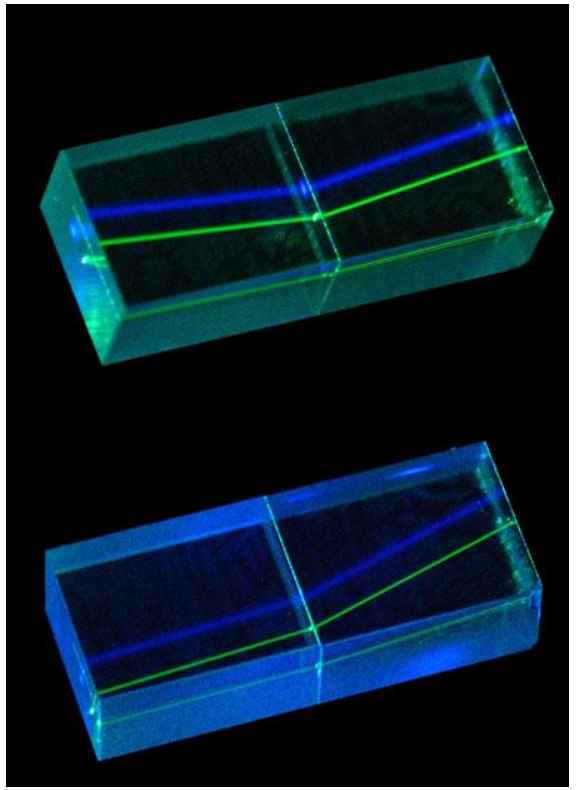
Recall : Refraction !





$n_1 \sin\alpha = n_2 \sin\beta$





What is the underlying principle ?

Principle of *least time of light*.

125 BC Hero of Alexandra

1650 Fermat

… out of all possible paths that it might take to get from one point to another, light takes the path which requires the shortest time.

R. Feynman

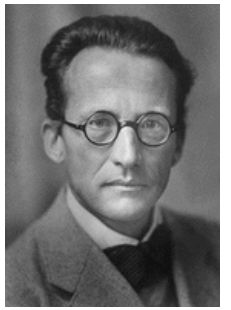
Path of the lazy man … Occam's Razor

How can we comprehend all these ?

Hamilton draw parallels between :
Optics and Mechanics

$$[\nabla L(r)]^2 = n^2(r)$$

$$[\nabla W(r)]^2 = 2m[E - V]$$



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Schrodinger took inspiration from the above

$$\nabla^2\psi(r) = -\frac{8\pi^2 m}{h^2}(E - V)\psi(r)$$

What is the **Quantity** of interest here ?

Aha ! what is Psi, ψ ?

Not Sigh !

Schrodinger (1926) solved the equation for the hydrogen atom but realized that ψ is a complex quantity … *unfortunately* ***i*** is embedded inside.

Suspected ψ is not a meaningful quantity … *cannot be measured.*

Suggested $\psi\,\psi^*$ … the weighted function

Eventually, $e\psi\psi^*(r)$ … interpreted as electronic charge density at distance *r.*

Recall: Schrodinger arrived at the famous wave equation for matter by pushing the analogy due to Hamilton between optics and mechanics (dynamics) via least action principle.

ψ is sometimes called "state" function.

Complex Number

"copy cat "

Recall the Quadratic Equation $ax^2+bx+c=0$

From Secondary School : The Solution is $x=\dfrac{-b\pm\sqrt{b^2-4ac}}{2a}$

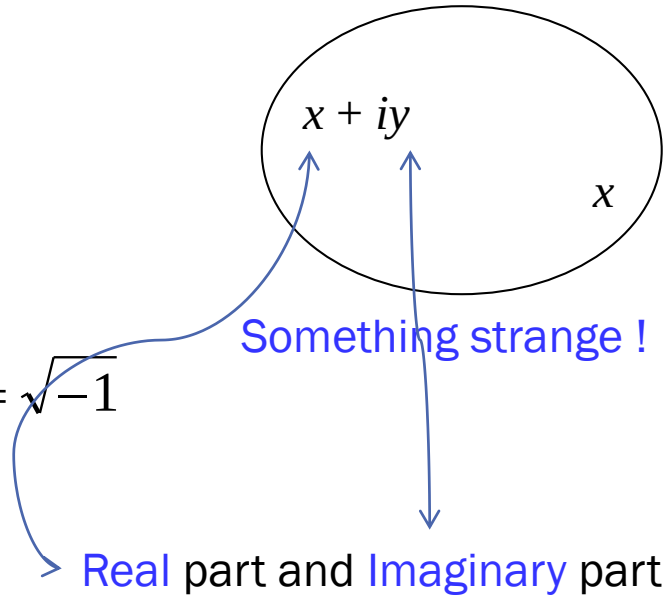
Example : Solve $x^2-2x+5=0$

$$x=\frac{2\pm\sqrt{-16}}{2}$$

$$=\frac{2\pm\sqrt{-1}\sqrt{16}}{2}$$

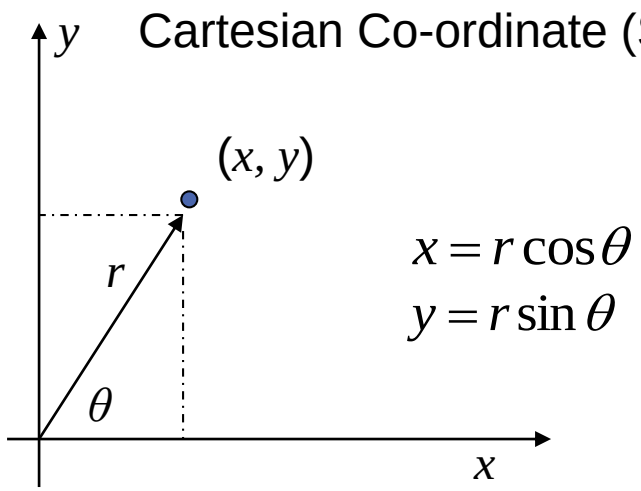
$$=1+2i \quad or \quad 1-2i$$

$i=j=\sqrt{-1}$



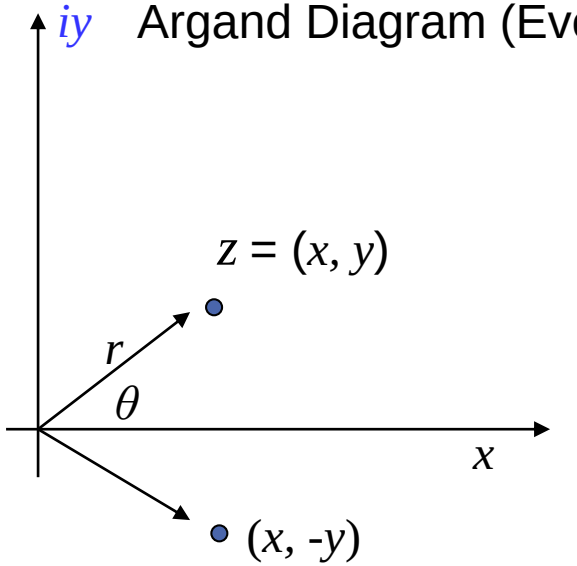
How do we visualize a complex number ?

Wonderful Complex Numbers



Cartesian Co-ordinate (Sec. Sch.)

$$x = r\cos\theta$$
$$y = r\sin\theta$$



Argand Diagram (Everyone)

$$z = x + iy$$
$$= r\cos\theta + ir\sin\theta$$

Note

z^* cousin

$z^* = x - iy$ (*conjugate*)

$r = |z|$ (*magnitude*)

Crown Jewel (Euler)

$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$e^{i\pi} + 1 = 0$$

What we want !

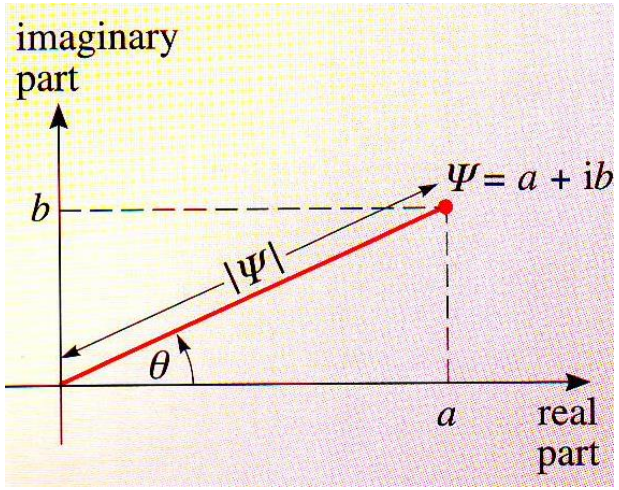
$$z^* z = |z|^2 \text{ Real number}$$

Why is this so? Work it out

Engineering

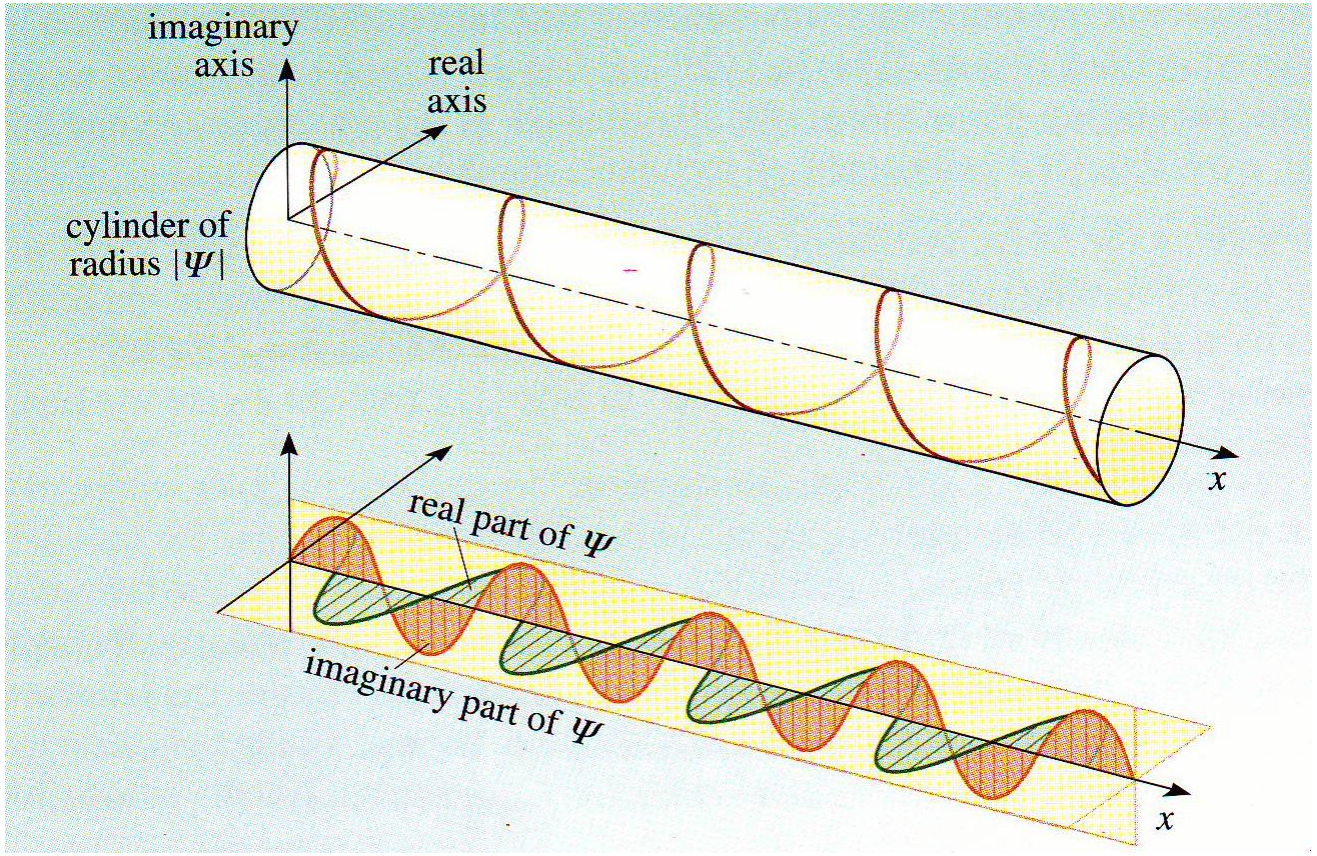
$$z = re^{i\theta}$$
$$= r\angle\theta$$

Possible Visualisation of Complex Numbers



$$\psi(x,t) = e^{i\theta}$$

$$= \cos\theta + i\sin\theta$$



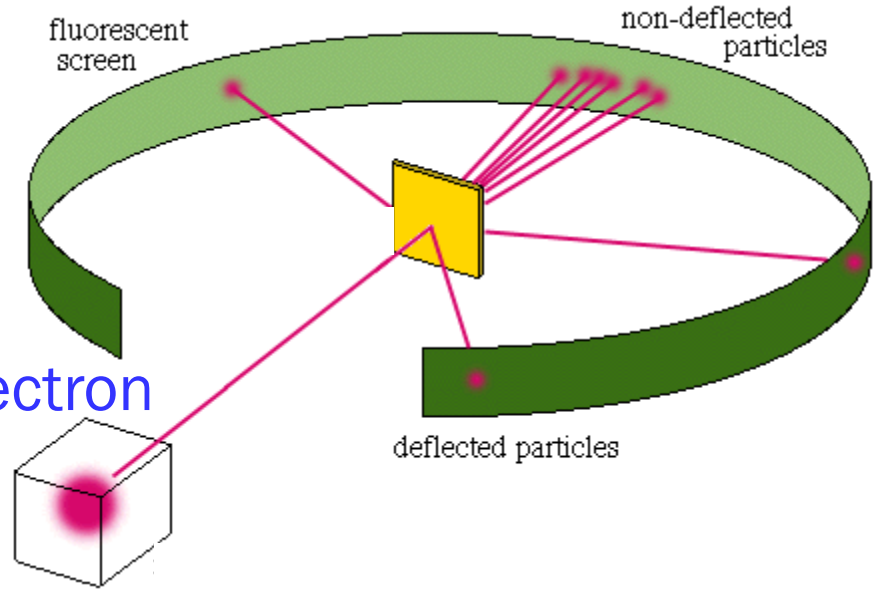
$$where\ \theta = \omega t - kx,\ r = 1$$

Born (Heisenberg's boss) "Scattered" thinking !

Heisenberg

cannot find for sure how the particles will be scattered

... sometimes here sometimes there ... !



Scattered electron

Born

4 days later … in a footnote

… ψ_{mn} determines the probability for the scattering of the electron from the z direction in the direction (θ, φ)…

ψ^2 The footnote that won a Nobel: A more precise consideration shows that *the probability is proportional to the* ***Square of*** ψ_{mn}.

So it was Born who realized that neither of these (few slides back) represent the probability and that only does.

Others : $|\psi|$ $|\psi^2|$

Did you see the oversight ?

$$\psi^* \psi = |\psi|^2$$

Lecture 11

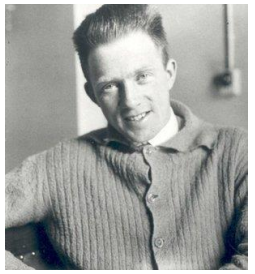
$$\langle \mathcal{L} | \hat{\mathcal{A}} | \mathcal{R} \rangle$$

Consider Left and Right Slits !

End of Determinism
Rise of Probabilistic Mother Nature

Oops !

Born declared:



One obtains the answer to the question, not “what is the state after the collision but how ***probable*** is a given effect of the collision” … I myself tend to give up determinism in the atomic world.

“ in those days he actually had no idea what a **matrix** was. It was he who reaped all the rewards of our work together, such as the Nobel Prize (1932)”.

Later 1954 Born won the Nobel Prize, Heisenberg said: “I was so relieved”

Applications of “Sigh (Psi)”

Bridge of Sighs

How can we comprehend all these ?

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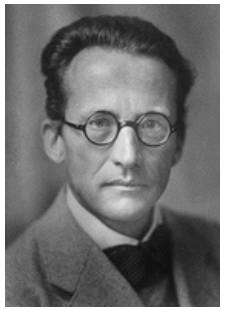
$$[\nabla W(r)]^2 = 2m[E - V]$$



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Schrodinger took inspiration from the above

$$\nabla^2\psi(r) = -\frac{8\pi^2 m}{h^2}(E - V)\psi(r)$$

What is the **Quantity** of interest here ?

How to apply Psi to the Bohr atom ?

For the electron in the hydrogen atom we now write it as ...

$\psi(x, y, z)$ or $\psi(r)$ sometimes called (*probability*) amplitude

There are *other labels* $\psi_{n,l,m_l}(x, y, z)$ to describe the ***state*** of the electron more completely ... *give up mini solar system !*

Schrodinger told us that the *wavefunction* $\psi(r)$ is a complex quantity and cannot be measured in any experiment but we need not lose heart. Born told us that one can certainly measure, the square of the absolute value of Psi because it has the meaning of probability ... *always* +ve !

$$\left|\psi_{n,l,m_l}(x, y, z)\right|^2$$

n : energy level
l : orbital angular momentum
m_l : orbital magnetic moment

Is there an Analogy ?

For the electron in the hydrogen atom we now write it as …

$\psi(x,y,z)$ or $\psi(r)$ sometimes called (probability) amplitude.

There are other labels $\psi_{n,l,m_l}(x,y,z)$ to describe the ***"state"*** of the electron more completely … ***give up mini solar system !***

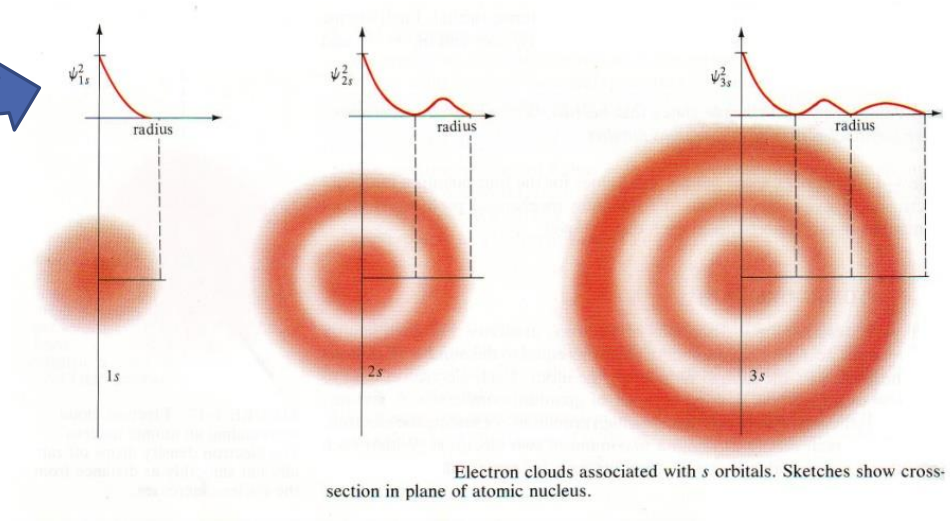
$$\psi_{n,l,m_l}(x,y,z)$$

State of the person

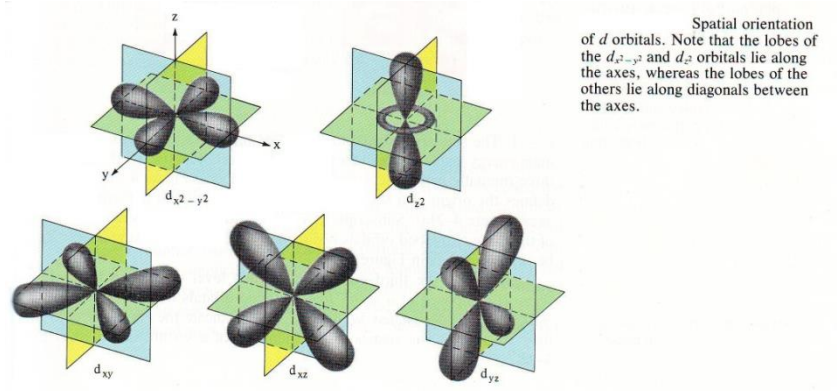
Happy, Angry, Melancholic, ?....? (place)

$|\psi_{n,l,m_l}|^2$ For Hydrogen Atom

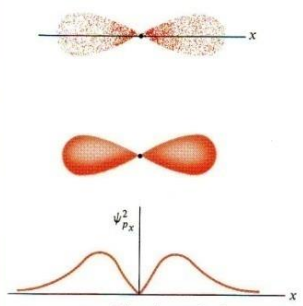
Hydrogensporbital.mov



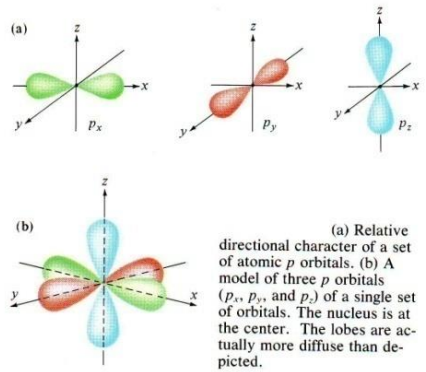
Electron clouds associated with *s* orbitals. Sketches show cross-section in plane of atomic nucleus.



Spatial orientation of *d* orbitals. Note that the lobes of the $d_{x^2-y^2}$ and d_{z^2} orbitals lie along the axes, whereas the lobes of the others lie along diagonals between the axes.



The shape of a 2*p* orbital—three representations.



(a) Relative directional character of a set of atomic *p* orbitals. (b) A model of three *p* orbitals (p_x, p_y, and p_z) of a single set of orbitals. The nucleus is at the center. The lobes are actually more diffuse than depicted.

So we have to give up the mini solar system idea introduced by Bohr !

Instead we find that the electron probability cloud forms beautiful and intricate patterns.

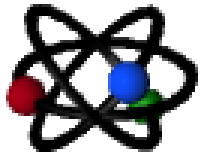
Depending on the values of n, l, m_l, the probability of finding the electron is more in some directions and less in others.

$$\psi_{n,l,m_l}(x,y,z)$$

So how is “sigh” or Psi connected to Bohr’s atomic mini solar system ?

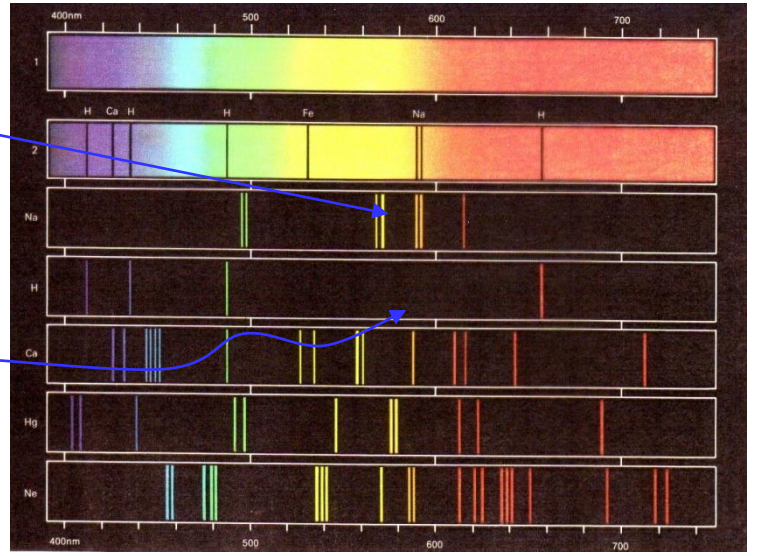
If you need a picture or analogy for your mind ? !

Niels Bohr Atoms

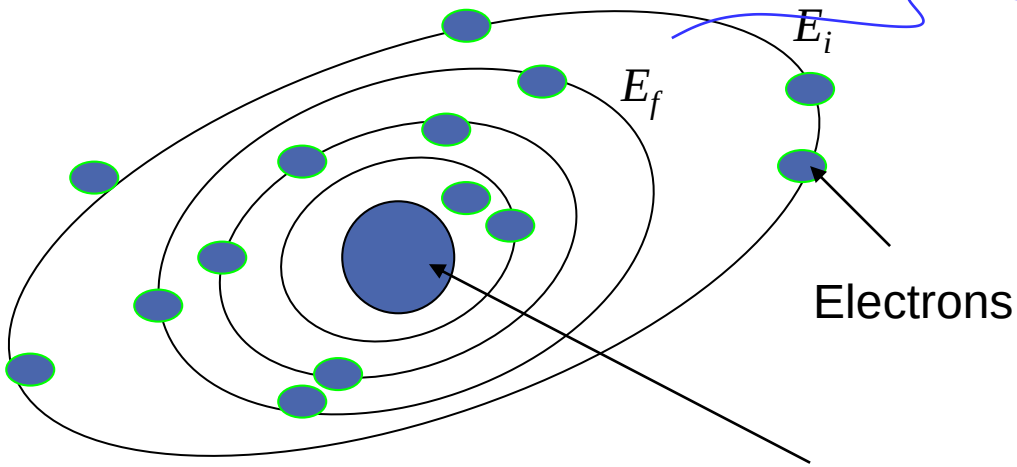


How Bohr's theory explain this ?

Bohr's Suggestion : "**Jumps up & down**" !



Bohr's Mini Solar System Model



Protons and Neutrons resides in the Nucleus … Nucleons

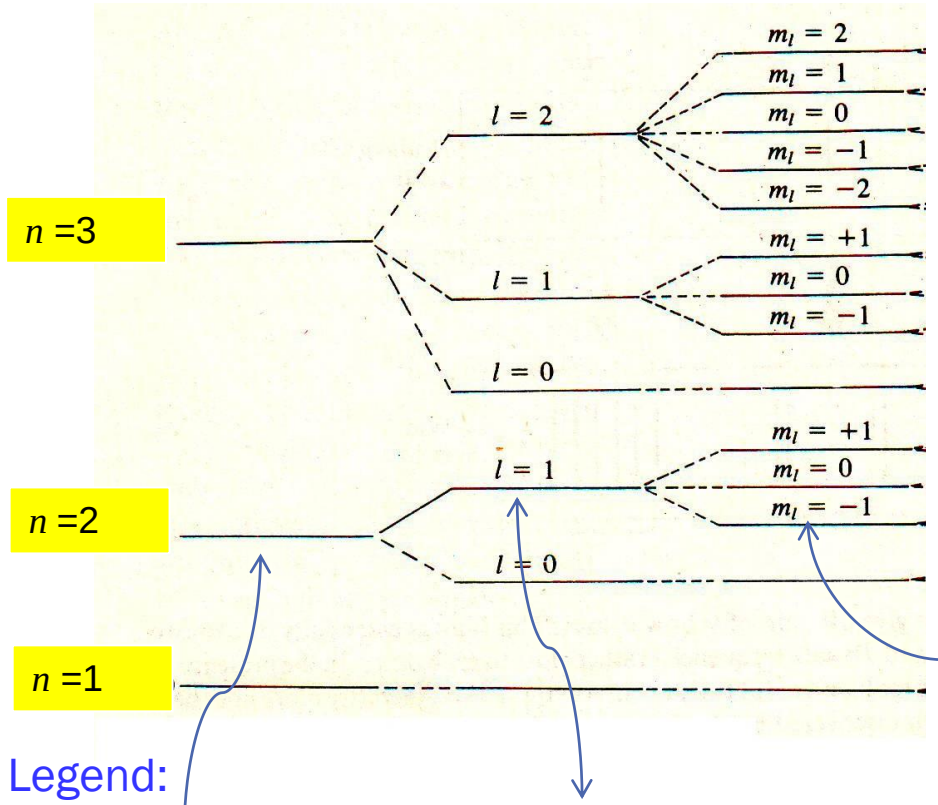
$$E_i - E_f = hf = E_g\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

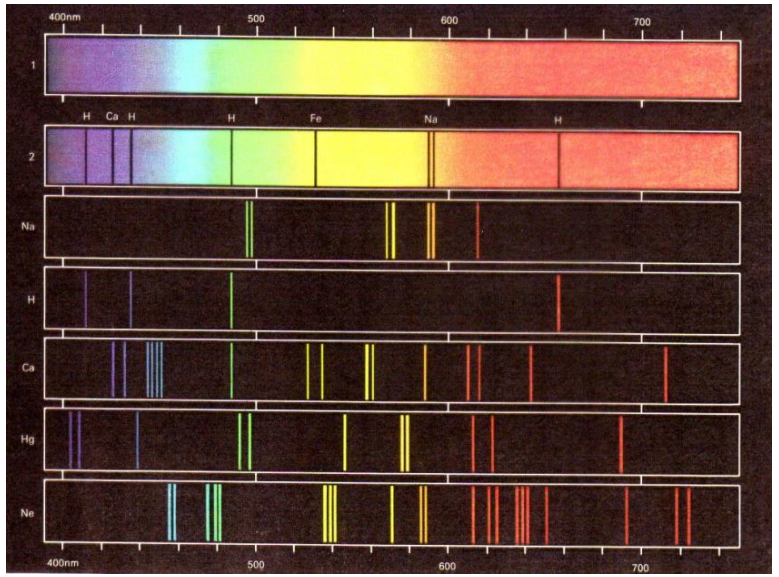
-13.6 eV … ground state energies

Note 1 : Negative value

Note 2: There is a value ? Why ?

$|\psi_{n,l,m_l}|^2$ Psi Labels





The psi needs 3 labels (or quantum numbers) to describe the electron.

Legend:

Orbit shell, orbital angular momentum, orbital magnetic quantum number or principal quantum number, orbital quantum number, orbital magnetic quantum number

A Socratic Question !

Why are videos and images of Atoms always seem to be fuzzy and electrons flying in all directions ?

$$\Delta x \Delta p \approx \hbar$$

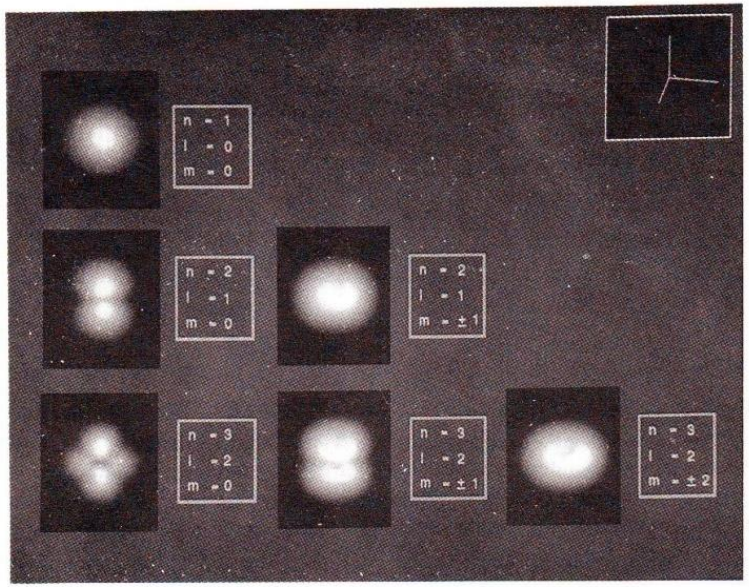
$$\Delta x \Delta mv \approx \hbar$$

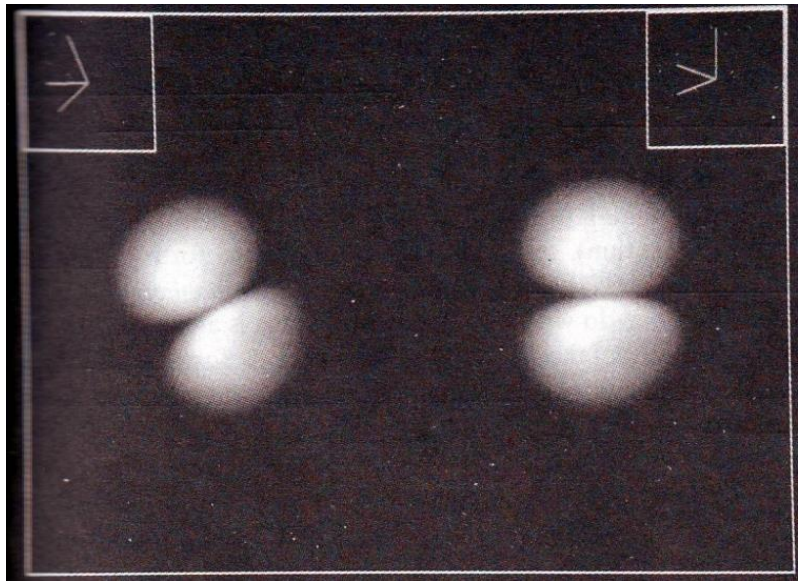
$$\Delta x \Delta v \approx \hbar / m$$

Another Socratic Question !

A good & fair question ?

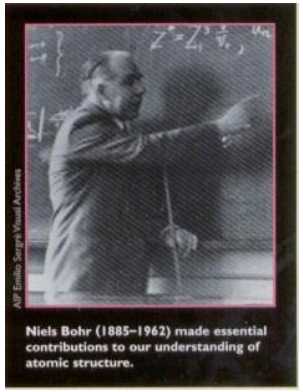
So how to take such orbital pictures ?





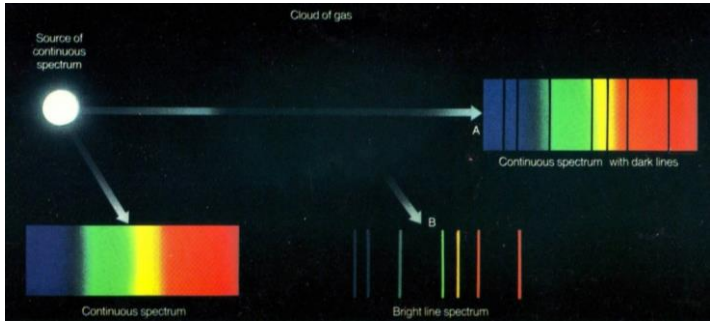
"I have personally met students who are majoring in chemistry or physics or math and believe that those pictures of orbitals you see in chemistry or physics book are shapes that have actually been measured or observed in some way. They are not. There is no scientific instrument that can directly measure the shape of an electron orbital. The reason is not merely that scientists just don't try hard enough. The reason is Heisenberg's Uncertainty Principle." *The bell that Rings Light*, D. Wallace & J Belbruno, Dartmouth College, USA

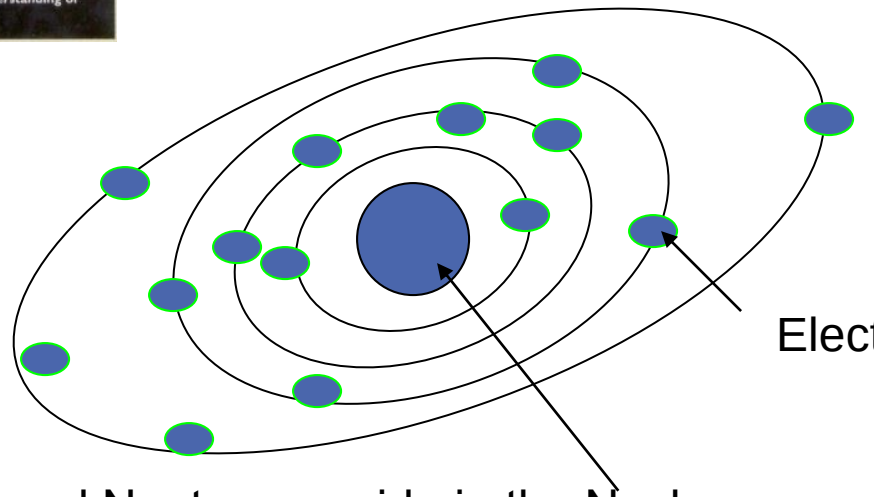
Niels Bohr



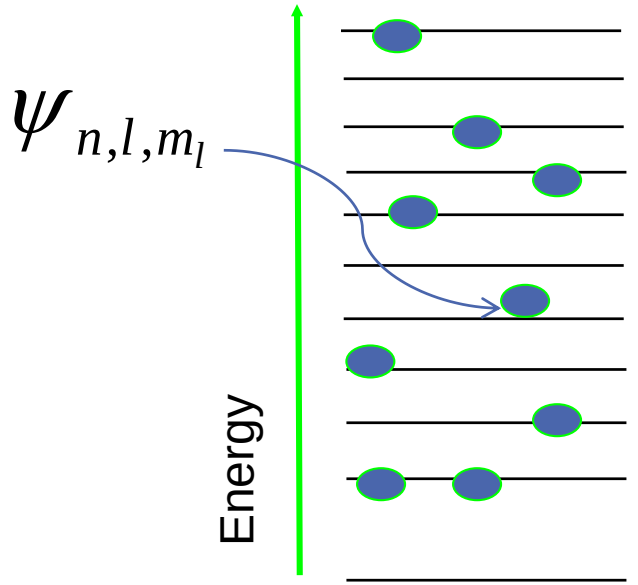
Absorption Spectra

Emission Spectra





Protons and Neutrons reside in the Nucleus … collectively called Nucleons.



More surprises ahead !

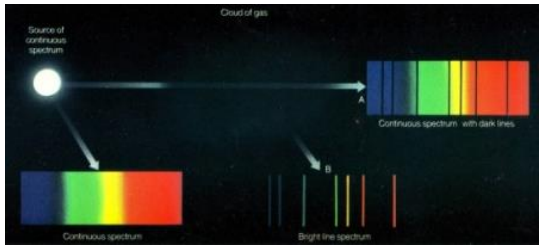
The message … no need a mental solar picture of the atom !

we persuade you to give it up !

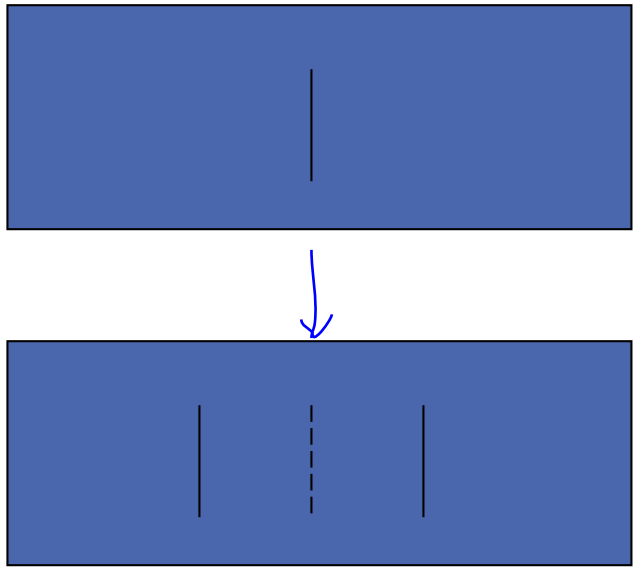
More surprises ahead !

More Blurs !

Zeeman Effect



Faraday did the splitting experiment to see if "blurred" spectra are affected by magnetic fields.



1896, Zeeman from Holland saw the broadened (blurred) lines

Lorentz

But Lorentz explained it using physics of that time.

The issue was settled ? ! ? !

Adding Spin

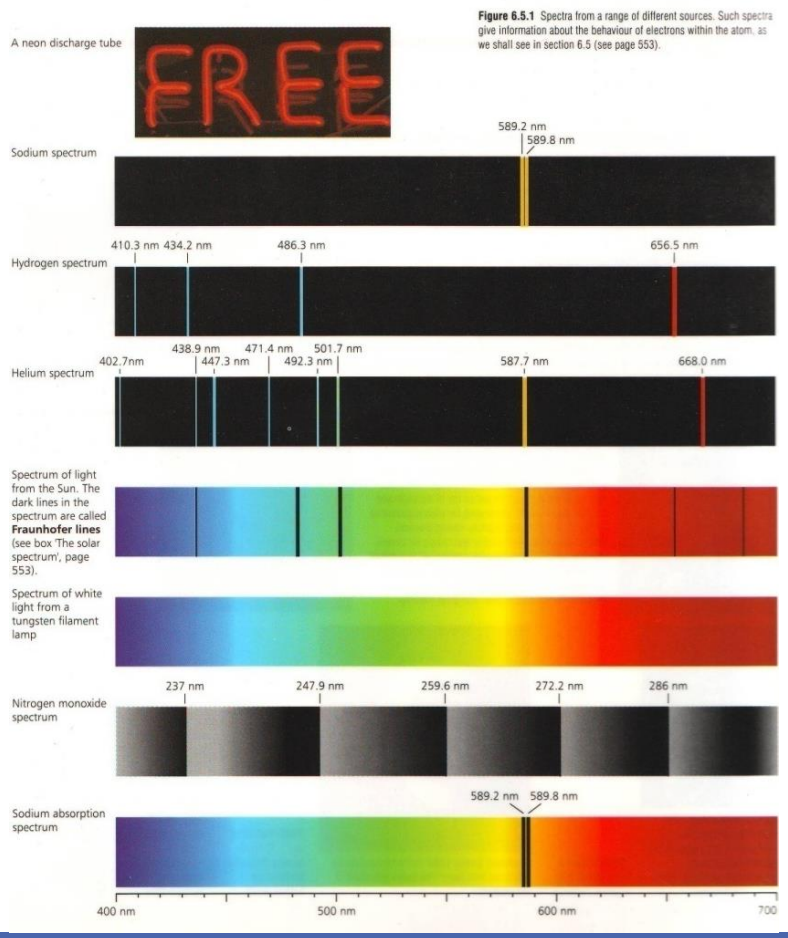
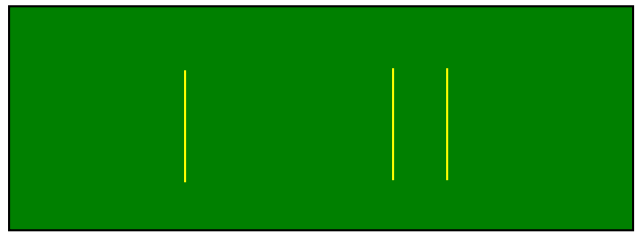
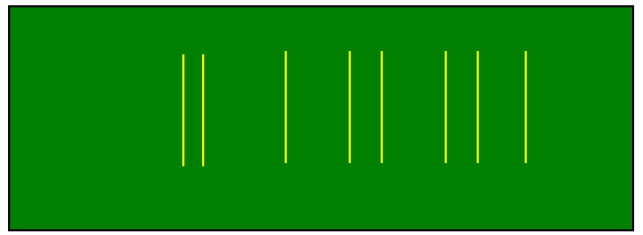


Figure 6.5.1 Spectra from a range of different sources. Such spectra give information about the behaviour of electrons within the atom, as we shall see in section 6.5 (see page 553).

Sodium Yellow D lines

No magnetic field





Lines split with magnet

Anomalous Zeeman effect cannot be explained by classical physics used by Lorentz.

Let us Spin !

Go back to the mini solar system; perhaps just like the earth, the electron is also spinning.

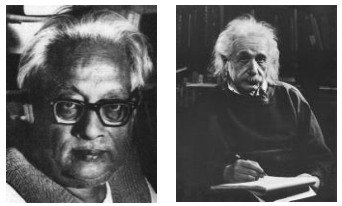
Uhlenbeck and Goudsmit studied the problem very carefully also came up with the idea of electron spin but ***with a twist*** …

realized that *it is not physically spinning* but possess a mysterious spin (angular momentum). Stern-Gerlach Experiment.

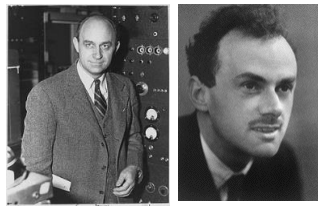
Oh No ! My head is spinning now !

A Socratic thought

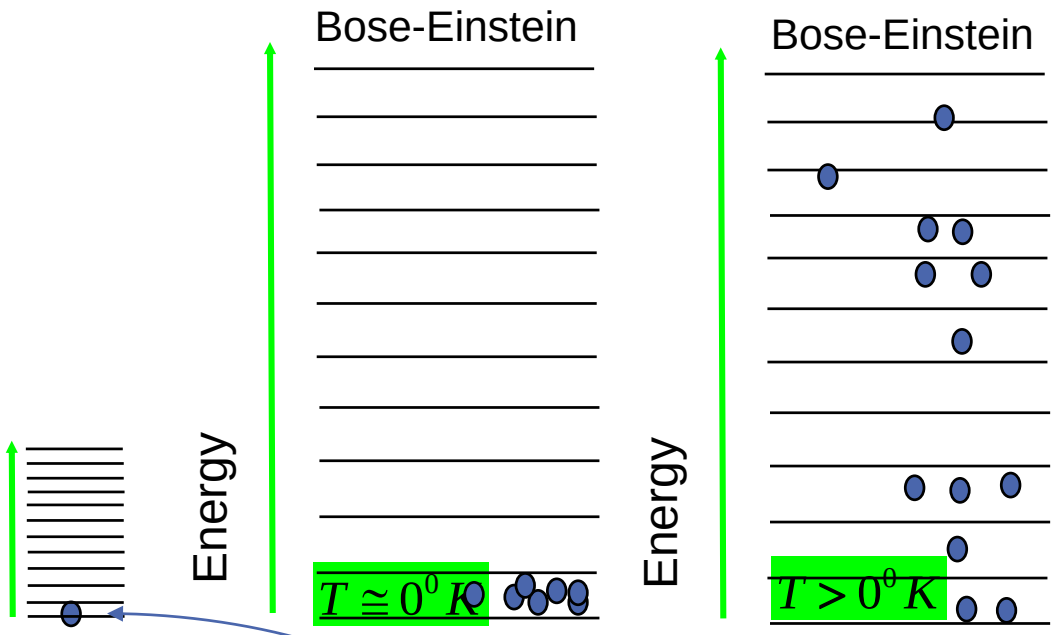
Spin is just a *label* !
Now we do know, “Spin” comes in 2 types only
Integer and Non-integer

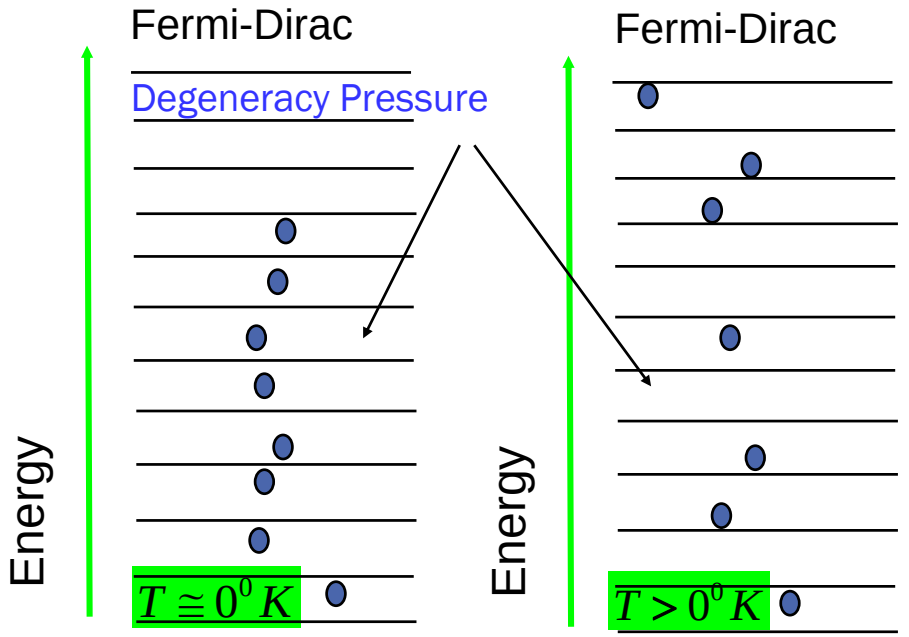


Bose Statistics



Fermion Statistics



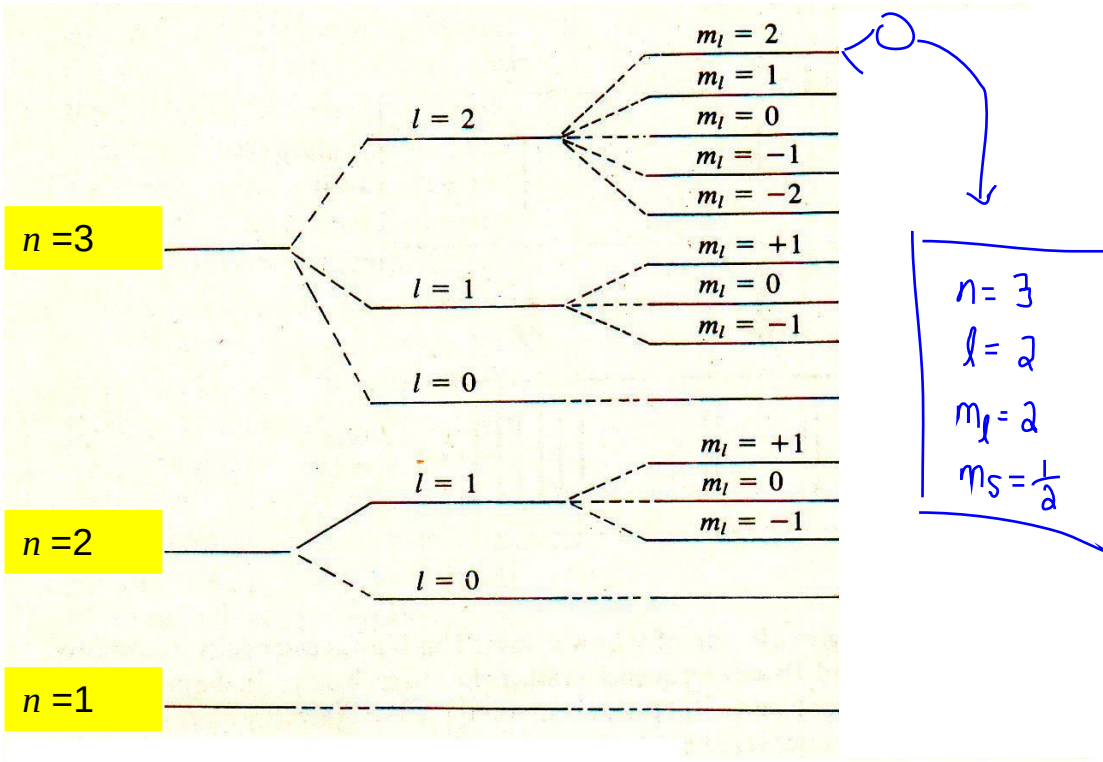


Note : At high temperature Bosons (Integer Spin) & Fermions (Half fractional Spin) behave like Boltzmann (Maxwell) particles. The micro-particles become so cold that the uncertainty in their position is comparable to the separation between micro-particles. This means that ~~that~~ several micro-particles can occupy the same region of space at the same time … they lose their individuality completely and behave as a single quantum entity … Bose Einstein Condensate … classical tennis balls cannot do this right !

So Spin is just a *label* !

If you still need a picture for where “Spin” fits into the atomic picture

How to "understand"? More labels $|\psi_{n,l,m_l,m_s}|^2$



Spin up(1/2) or Spin down(-1/2)

Electron State ψ_{n,l,m_l,m_s}

How to know how many energy levels? (2*x* + 1) number of levels, *x* = *l* or s

After the discovery of the electron spin, we now need 3 + 1 = 4 labels (or quantum numbers) to describe the electron. This Spin did not come from solving the Schrodinger equation. It is a special kind of Spin (*intrinsic*).

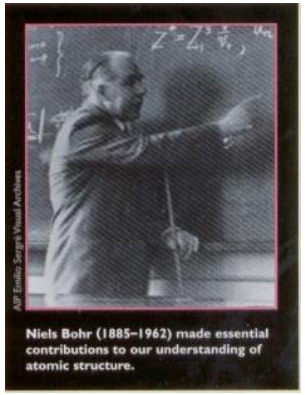
Socratic Question
So where does Spin come from ?
Why up and down ?

Can you think about it ?

Answer : 3 words only

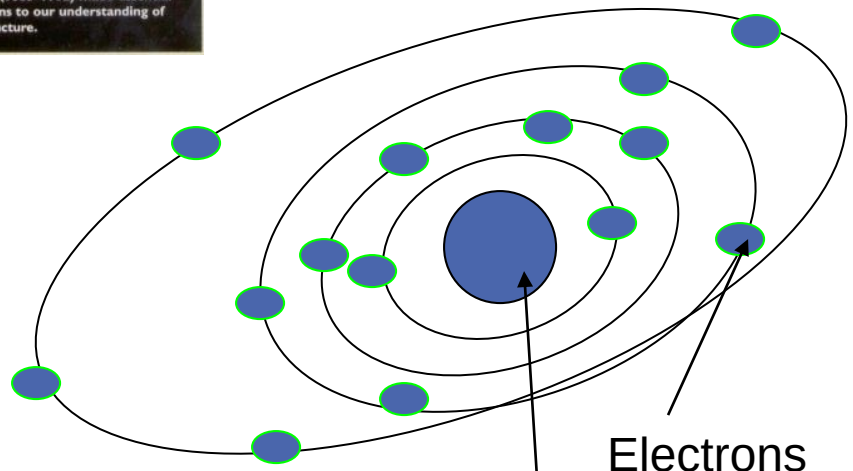
So how can we picture an atom in our minds !

Niels Bohr

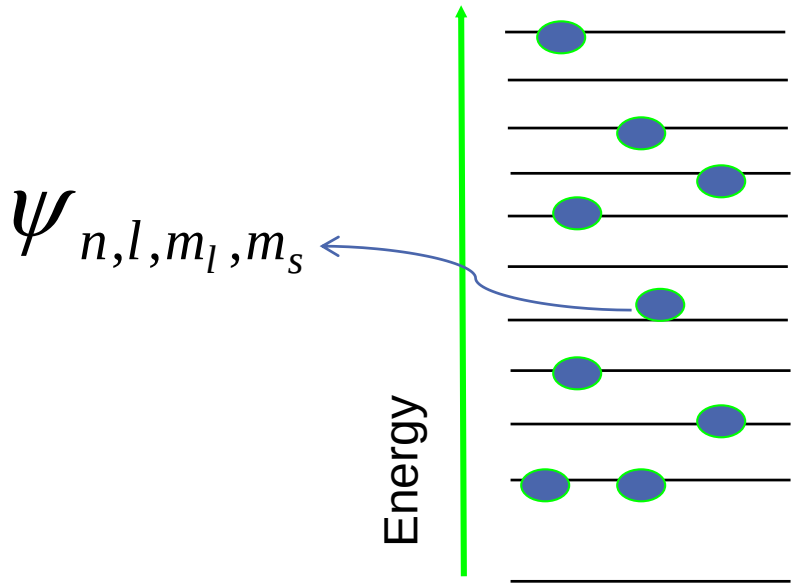


Absorption Spectra

Emission Spectra

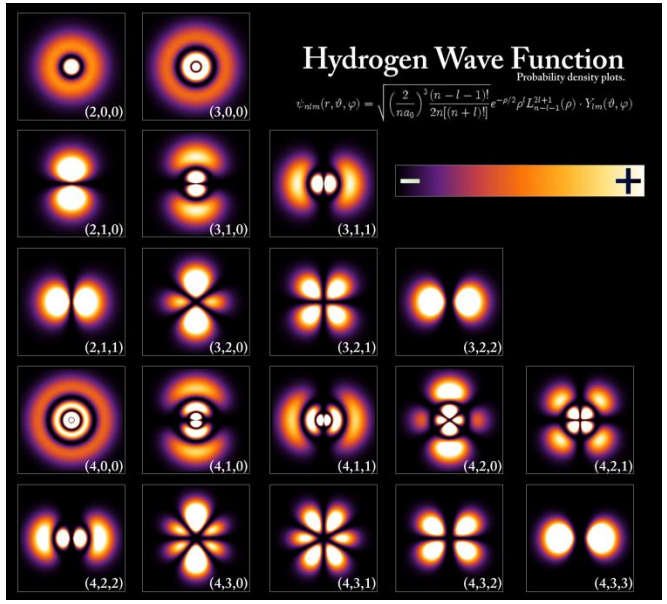


Protons and Neutrons reside in the Nucleus … collectively called Nucleons.



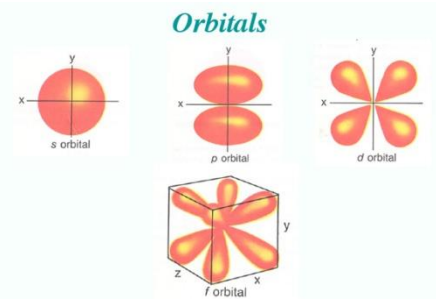
Where to find the electron ?

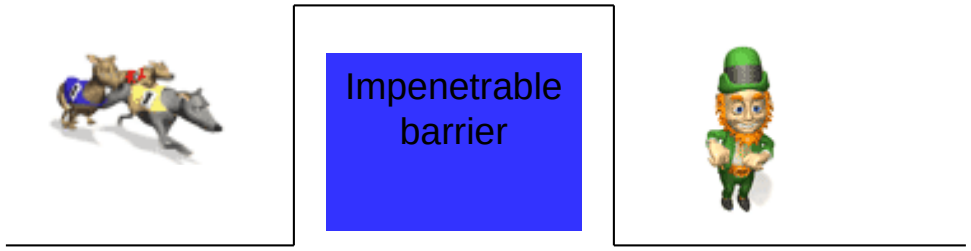
$$\left|\psi_{n,l,m_l,m_s}\right|^2 = \psi^*\psi$$



One more surprising result ! Tunneling

Quantum Tunneling





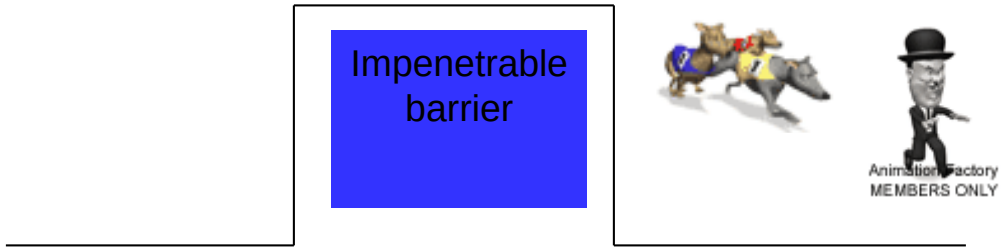
No way for Tunneling in classical Newtonian Mechanics

Strange 2

Consider the tennis ball I always show you.

Strangely, in QM calculation for the tennis ball, there is a probability for the ball to emerge on the other side of the wall. There is a finite value though very small, but it is not zero.

Strange 1



This Quantum Mechanical Tunneling : Example: Radioactivity: tunneling / randomly

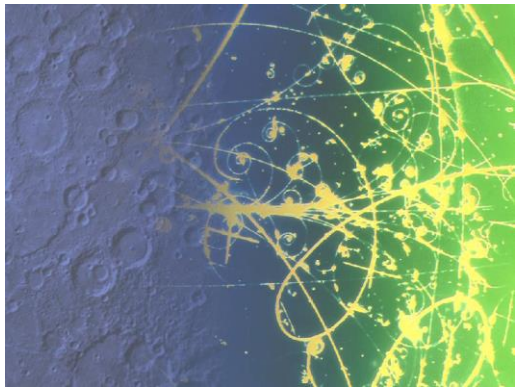
Examples of Quantum Tunneling

It turns out that even in biology it is now well established that electrons quantum tunnel in enzymes, allowing certain chemical processes to speed up by several orders of magnitude …

… exploring over the past few years is whether quantum tunnelling of hydrogen nuclei (protons) in the form of a hydrogen bond has a role to play in one of the most important processes in molecular biology: DNA mutation
… spontaneous mutation – a change in the genetic code, for example from ATCAT to ATCAC.

Jim Al-Khalili
Nature's quantum subways
Physics World March 2013

J. McFadden & J. Al-Khalili, *Life on the Edge : Quantum Biology* (2014)
Schrodinger, *What is Life* ? Cambridge U. Press (1944, 12th printing, 2012)



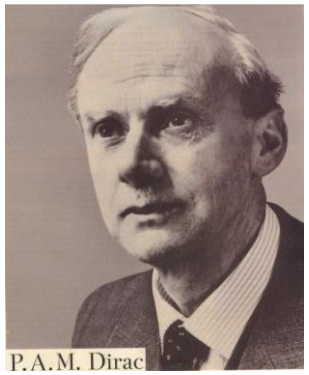
I cannot believe that God plays Dice. A. Einstein

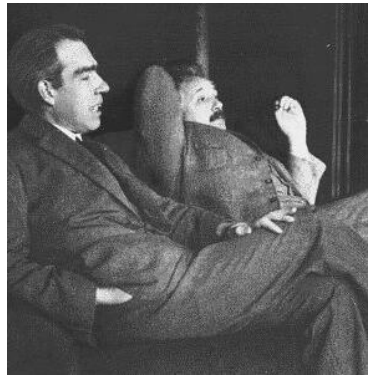
After the foundations of Quantum Mechanics were laid down …

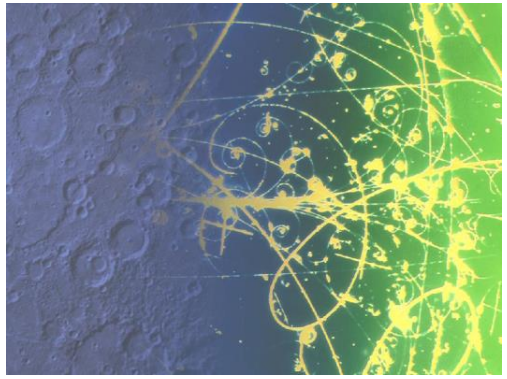
… It was a time when 2nd-rate men did 1st - rate work. Why ?

P. Dirac

Nobel Laureate, 1902 – 1984







More surprises ahead !

The final message … no need a mental solar picture of the atom ! we persuade you to give it up !

This is the Reality !

We cannot make the mystery go away by explaining how it works. All that can be done is to tell you how it works; that is the way with Quantum Physics.

R. Feynman

Historically, the electron was thought to behave like a particle and then it was found that in many respect it behaved like a wave. So it really behaves like neither. Now we have given up. We say: it is like neither.

R. Feynman

There is no quantum world. There is only an abstract quantum mechanical description. It is wrong to think that the task of Physics is to find out how Nature is. Physics concerns what we can say about Nature.

N. Bohr

Heisenberg's approach

An atom would be represented not by a physical picture, but by *a purely mathematical model.* Instead of thinking about electron orbits one could think of the atomic model as a matrix with row an columns of empty spaces. Each space would be filled a number as we obtained the necessary information about the particular atom.

Applying one matrix to another in a certain defined way would give a set of numbers representing the results of experimental observation. For example, apply the 'frequency matrix' to the hydrogen matrix would give the observed values of the frequencies of light emitted by hydrogen. Apply the same frequency matrix to the matrix for the sodium atom would give the special lines emitted by sodium, and so on.

The Development of Quantum Mechanics
Alex Montwill & Ann Beslin (2008)

Is there a real world out there?

What we observe **is not nature itself**, but nature exposed to our method of questioning."

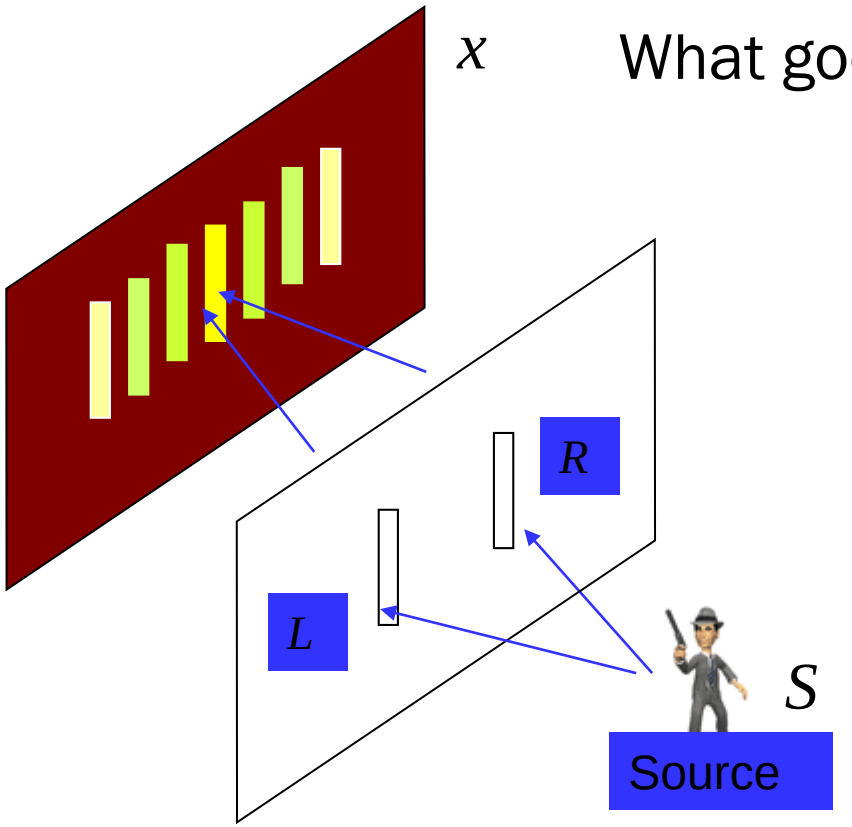
Heisenberg

Perhaps this is what we mean by "understanding" nature at its most fundamental level !

Finally 2 slits experiment

Revisit

What is Psi in our 2 Slits ?



What good are State labels ?

$$\langle x|s\rangle = \langle x|s\rangle_L + \langle x|s\rangle_R$$

But we can also write

$$\langle x|s\rangle_L = \langle x|L\rangle\langle L|s\rangle$$

$$\langle x|s\rangle_R = \langle x|R\rangle\langle R|s\rangle$$

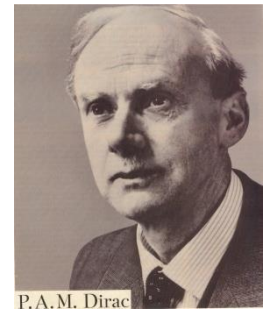
In General

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

Echoes a new idea : 1) Principle of Superposition !

What is the emphasis ? 2) States

Theory of Bras & Kets



$\langle x | s \rangle$

A related idea for the symbol : Conditional probability

$$P(x|s) = \frac{P(x \cap s)}{P(s)}$$

$P(A|B)$ Bayes' Theorem

Means event x given event s

But Where is Psi ? $\psi = \langle x | s \rangle = \psi_L + \psi_R$

photons can be in both L & R at the same time

Is there a real world out there?

The exact sciences also start from the assumption that in the end it will always be possible to understand nature, even in every new field of experience, but that we may make no a priori assumptions *about the meaning of the word* ***"understand"***.

Heisenberg

??????????????

Perhaps this is what we mean by "understanding" nature at its most fundamental level !

Is there a real world out there?

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