

PH101: Physics 1

Module 3: Introduction to Quantum Mechanics

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Contents

Quantum Mechanics: Two-slit experiment. De Broglie's hypothesis. Uncertainty Principle, wave function and wave packets, phase and group velocities. Schrödinger Equation. Probabilities and Normalization. Expectation values. Eigenvalues and eigenfunctions.

Applications in one dimension: Particle in a box, Finite Potential well, Harmonic oscillator.

Text / References:

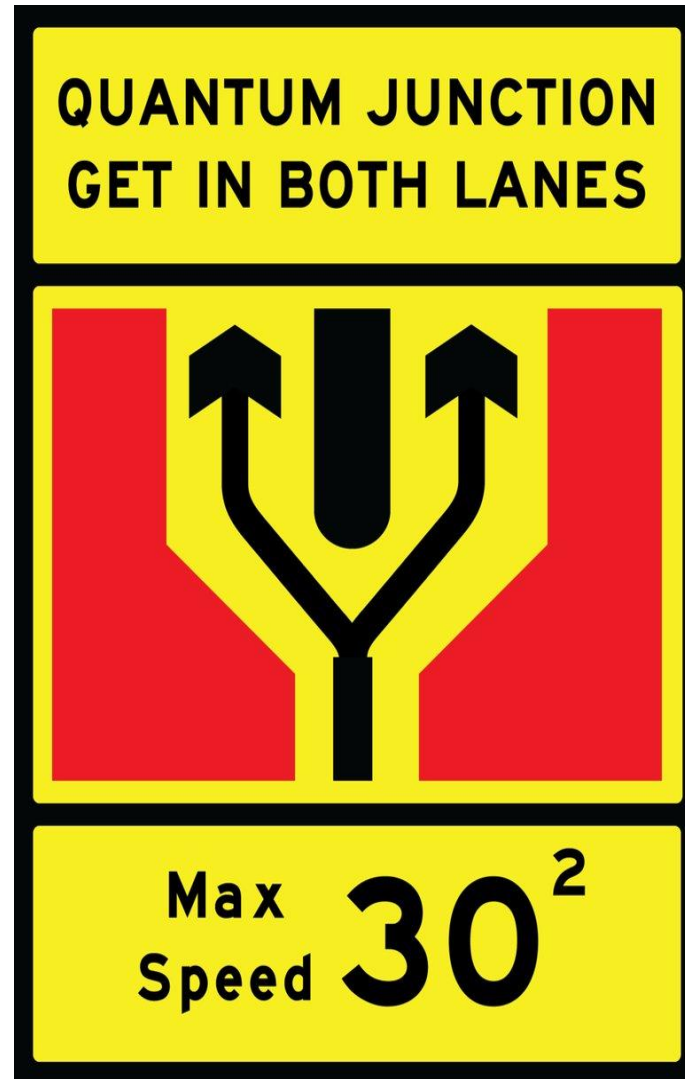
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Introduction to Quantum Mechanics

“If you see a fork in the road in front, you take it!”

American baseball player Yogi Berra’s joke which applies well to describe the approach to quantum mechanics.

Yogi Berra [1925-2015] was America’s Navjot Singh Sidhu who combined sporting excellence and witty (and sometimes questionable) humour.



$$|\psi\rangle = \frac{1}{\sqrt{2}}|R\rangle + \frac{1}{\sqrt{2}}|L\rangle$$

The above equation is a mathematical description of the probabilistic nature of Quantum Mechanics

Historical Introduction: The drawbacks of classical physics

Despite great success in explaining physical phenomena, the classical period of physics [antiquity-1900] which saw the development of Newtonian mechanics, Electromagnetic theory (along with wave theory of light) and Statistical Mechanics and Thermodynamics was beset with conceptual difficulties by 1900, chief among them were –

- Electromagnetic theory and Statistical physics together predicted that hot objects at temperature T should emit radiation of various frequencies such that the intensity of radiation [dI in Joules per sq. meter per sec.] emitted between frequencies ν and $\nu + d\nu$ is (k_B is Boltzmann's constant and c is speed of light)

$$dI = \frac{2 \nu^2 k_B T}{c^2} d\nu$$

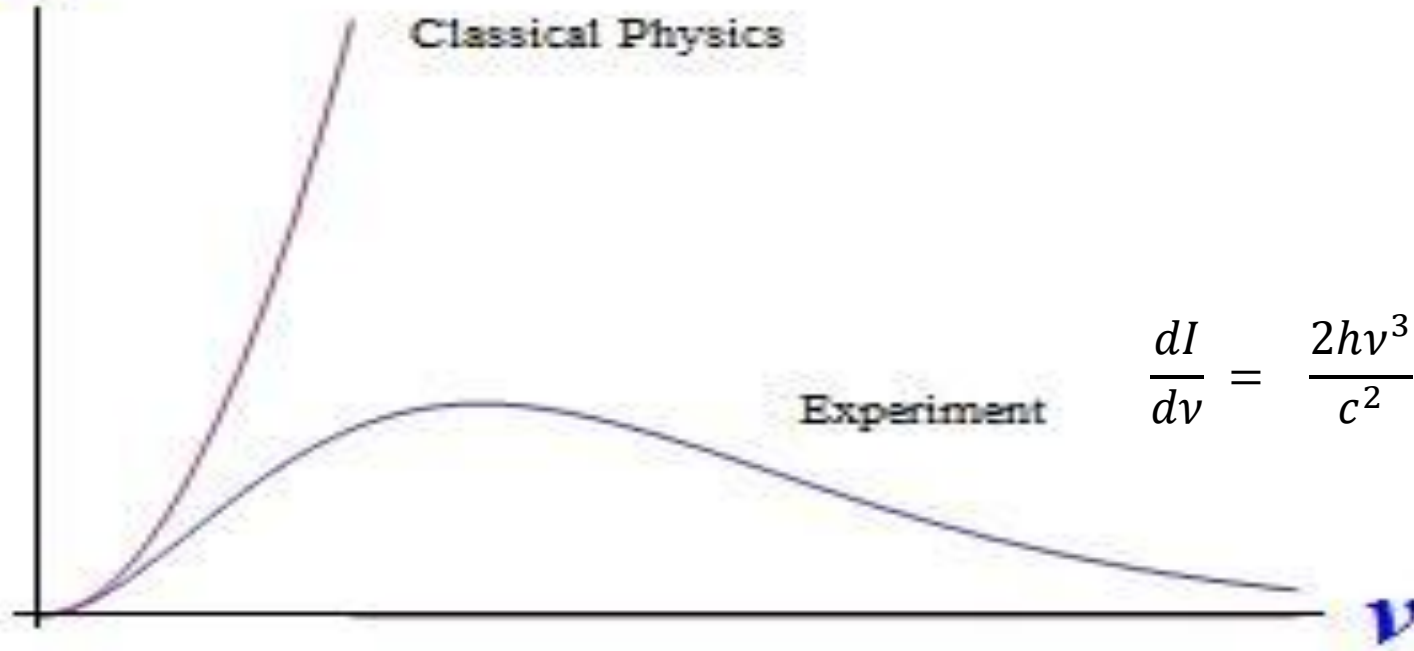
Read Ch.1 of R. Eisberg, R. Resnick

An accurate way of measuring this is to heat a large closed enclosure and pierce a small hole at the side and measure the radiation coming out – this is called “**black body radiation**”. The above theoretical answer meant that the total intensity emitted by the object for all frequencies is infinite! This is called the ultraviolet catastrophe which shows there is something seriously wrong with the above answer.

Experiments told a different story. By the 1890's, experimental techniques had improved sufficiently that it was possible to make fairly precise measurements of the energy distribution in this black body radiation. In 1895, at the University of Berlin, Wein and Lummer punched a small hole in the side of an otherwise completely closed oven, and began to measure the radiation coming out.

$$\frac{dI}{d\nu}$$

$$\frac{dI}{d\nu} = \frac{2 \nu^2 k_B T}{c^2}$$



Planck's curve fitting guess for the experimental curve

$$\frac{dI}{d\nu} = \frac{2h\nu^3}{c^2} \frac{1}{e^{\frac{h\nu}{k_B T}} - 1}$$

On 19 October 1900 the Berliner, Max Planck (age 42) announced a formula that fit the experimental results perfectly, yet he had no explanation for the formula -- it just happened to fit. He worked to find an explanation through the late fall and finally was able to derive his formula by assuming that the atomic “jigglers” in the walls of the cavity which were thought to be emitting the radiation could not take on any possible energy, but only certain special “allowed” values. He announced this result on 14 December 1900. This date is now considered the birthday of quantum mechanics but at the time no one found it particularly significant.

The old quantum theory

Although the ideas of Planck did not take the world by storm, they did develop a growing following and were applied to more and more situations. The resulting ideas, now called "old quantum theory", were all of the same type: Classical mechanics was assumed to hold, but with the additional assumption that only certain values of a physical quantity (the energy, say, or the projection of a magnetic arrow) were allowed. Any such quantity was said to be "quantized". The trick seemed to be to guess the right quantization rules for the situation under study, or to find a general set of quantization rules that would work for all situations.

In 1911, Ernest Rutherford (age 40), a New Zealander doing experiments in Manchester, England, discovered **the atomic nucleus** -- only at this relatively late stage in the development of quantum mechanics did physicists have even a qualitatively correct picture of the atom! In 1913, Niels Bohr (age 28), a Dane who had recently worked in Rutherford's laboratory, introduced quantization ideas for the hydrogen atom. His theory was remarkably successful in explaining the colors emitted by hydrogen glowing in a discharge tube, and it sparked enormous interest in developing and extending the old quantum theory.

This success of the Bohr atom also resolved a paradox that Rutherford's description of a neutral atom – positive charged point-like nucleus and negatively charged electrons – posed. The electrons could not be static then that would make atoms unstable. Electrons somehow had to be revolving around the positively charged nucleus much like planets around the sun. But electromagnetic theory says accelerating charges radiate and the electron should spiral and fall into the nucleus. A calculation of this gives the lifetime of an atom with the observed size of orbits as 10^{-11} sec .

The year 1905 was an extraordinary year in the history of physics. Never before or since have so many profound ideas come out and that too from one individual – Albert Einstein

Einstein published four landmark papers that year which included

Read Ch.2 of R. Eisberg, R. Resnick

- a) An explanation of the photoelectric effect through the introduction of energy quanta for light
- b) Explanation of Brownian motion through statistical methods
- c) Development of Special Relativity
- d) Proof of energy and mass equivalence

Of these four, the work that had the most impact on the development of quantum theory was the first one in the form of this paper

Einstein, Albert (1905) *Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt, Annalen der Physik 17 (6): 132–148*

Translation: *On a Heuristic Viewpoint Concerning the Production and Transformation of Light*

New quantum theory – Quantum Mechanics

With the end of the First World War in 1918, work in quantum mechanics expanded rapidly. Many theories were suggested and many experiments performed. To cite just one example, in 1922 Otto Stern and his graduate student Walther Gerlach (ages 34 and 23) performed their important experiment that demonstrated quantization of angular momentum. Jagdish Mehra and Helmut Rechenberg, in their monumental history of quantum mechanics, describe the situation at this juncture well:

“At the turn of the year from 1922 to 1923, the physicists looked forward with enormous enthusiasm towards detailed solutions of the outstanding problems, such as the helium problem and the problem of the anomalous Zeeman effects. However, within less than a year, the investigation of these problems revealed an almost complete failure of Bohr's atomic theory.”

Thus the old quantum theory gave way to the modern Quantum Mechanics

Wave-particle duality : de Broglie relation

Louis de Broglie [1892 – 1987] was a French physicist who made ground breaking contributions to quantum theory. In his 1924 PhD thesis he postulated the wave nature of electrons and suggested that all matter has wave properties. This concept is known as the de Broglie hypothesis, an example of wave-particle duality, and forms a central part of the theory of quantum mechanics.

De Broglie won the Nobel Prize for Physics in 1929, after the wave-like behaviour of matter was first experimentally demonstrated in 1927.

"The fundamental idea of [my 1924 thesis] was the following: The fact that, following Einstein's introduction of photons in light waves, one knew that light contains particles which are concentrations of energy incorporated into the wave, suggests that all particles, like the electron, must be transported by a wave into which it is incorporated... My essential idea was to extend to all particles the coexistence of waves and particles discovered by Einstein in 1905 in the case of light and photons."
"With every particle of matter with mass m and velocity v a real wave must be 'associated'", related to the momentum by the equation:

$$\lambda = \frac{h}{p} \quad \text{where} \quad p = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Getting a feel for the wave nature of matter

Q. Find the wavelength of the matter wave associated with a tennis ball moving at 110 km/h

A. First, $v \ll c$ so that, $p \approx m_0 v$ Take the mass of the tennis ball to be $m_0 \approx 58 \text{ g}$

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34} \text{ J.s}}{58 \times 10^{-3} \text{ kg} \times 110 \times 10^3 \text{ m}/(3600 \text{ s})}$$
$$= 3.73881 \times 10^{-34} \text{ m}$$

Compare this with the size of the hydrogen atom

$$= 53 \times 10^{-12} \text{ m}$$

The de Broglie wavelength of a tennis ball can be taken to be zero. This means a tennis ball has negligible wave-like properties.

Q. Find the wavelength of the matter wave associated with an electron moving at 110 km/h

A. First, $v \ll c$ so that, $p \approx m_0 v$

$$\lambda = \frac{h}{p} = \frac{hc}{pc} = \frac{hc}{(m_0 c^2) \left(\frac{v}{c}\right)}$$

$$hc = 1.24 \text{ eV} \cdot \mu\text{m}$$

$$m_0 c^2 = 0.511 \text{ MeV}$$

$$\frac{v}{c} = 10^{-7}$$

$$\lambda = 24.3 \mu\text{m}$$

The typical size of a bacterium is $6 \mu\text{m}$.

$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$

Getting a feel for the particle nature of waves

Q. Waves on a rope have a wavelength of 10 cm. Find the momentum corresponding to a particle description of these waves. Given that the mass of the rope is 500g what is the speed of this “particle” ?

A.

$$p = \frac{h}{\lambda} = \frac{6.626 \times 10^{-34} \text{ J.s}}{0.1 \text{ m}} \\ = 6.626 \times 10^{-33} \text{ kg.m/s}$$

The speed is $v = 1.32 \times 10^{-32} \text{ m/s}$ which is imperceptible with current technology.

Q. In an electron diffraction experiment, the wavelength of the (matter wave corresponding to) electrons are measured to be $10 \text{ } \mu\text{m}$. Find the speed of the electrons.

A.

$$pc = \frac{hc}{\lambda} = \frac{1.24 \text{ eV}\mu\text{m}}{10 \mu\text{m}} = 0.124 \text{ eV}$$

But,

$$pc = m_0 v c = m_0 c^2 \left(\frac{v}{c} \right) = 0.511 \text{ MeV} \left(\frac{v}{c} \right)$$

Hence,

$$\frac{v}{c} = 2.43 \times 10^{-7} \text{ or } v = 73 \text{ m/s}$$

Classically, we may think of Planck's constant as vanishingly small.

$$\text{As } h \rightarrow 0$$
$$\text{Quantum Physics} \rightarrow \text{Classical Physics}$$

For the de Broglie relation this means,

$$p \lambda = h \rightarrow 0$$

This means, in the classical world,

a) If the particle property (momentum p) is not zero, the wave property (wavelength λ) has to be zero.

conversely,

b) If the wave property (wavelength λ) is not zero, the particle property (momentum p) has to be zero.

This means in a classical world, there are particle or waves. One entity cannot be both.

If you want to perceive speed, mass, wavelength etc. as a human observer with no special instruments all these quantities have to be in a window around the value 1 in the natural system of units (e.g. MKS) e.g. everyday speeds are between 0.001m/s and 1000m/s, masses you see around you are between 0.001 kg and 1000 kg e.t.c. Given this we can see that the smallness of Planck's constant compared to everyday scales means that according to de Broglie relation only microscopic objects will have particle and wave nature together in a proportion that can be seen with human senses.

$$p \lambda = m v \lambda = h$$

or,

$$v \lambda = \frac{h}{m}$$

To observe wave and particle properties of an object together using just human senses we have to ensure that $0.001 \text{ meter/s} < v < 1000 \text{ meter/s}$ and $0.001 \text{ meter} < \lambda < 1000 \text{ meter}$. Due to the smallness of Planck's constant this means the object has to have a mass in the range, $6.626 \times 10^{-40} \text{ kg} < m < 6.626 \times 10^{-28} \text{ kg}$. This means the object has to be a subatomic particle.

Hence in a classical world, something is either a wave or a particle but not both at the same time. But in the quantum world, every particle has wave-like property (even if it is negligible sometimes) and every wave has particle-like properties. Which aspect manifests itself, depends on the kind of measurements that are being performed.

Understanding particle & wave nature

Experiment with a gun (bullets as particles):

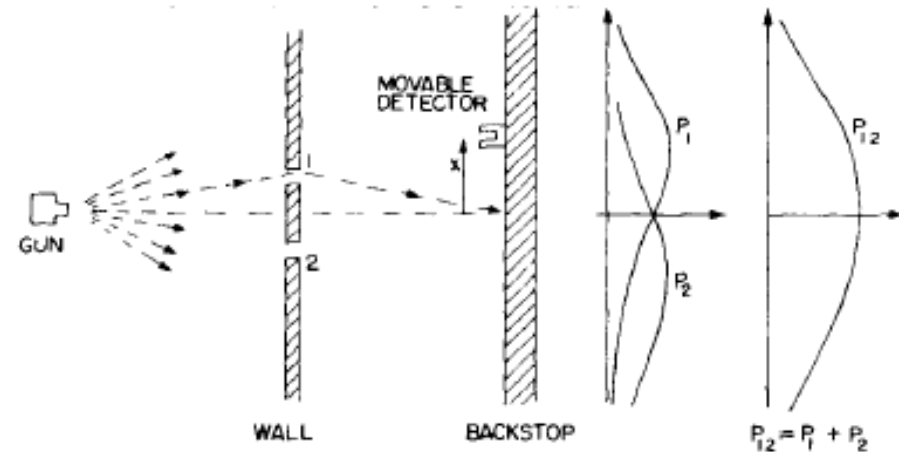
Detector counts number of bullets.

P_1 : probability when hole 2 is closed.

P_2 : probability when hole 1 is closed.

P_{12} : probability when both holes are open.

Result: No interference.



Experiment with water wave:

Detector records intensity of the wave.

I_1 : intensity when hole 2 is closed.

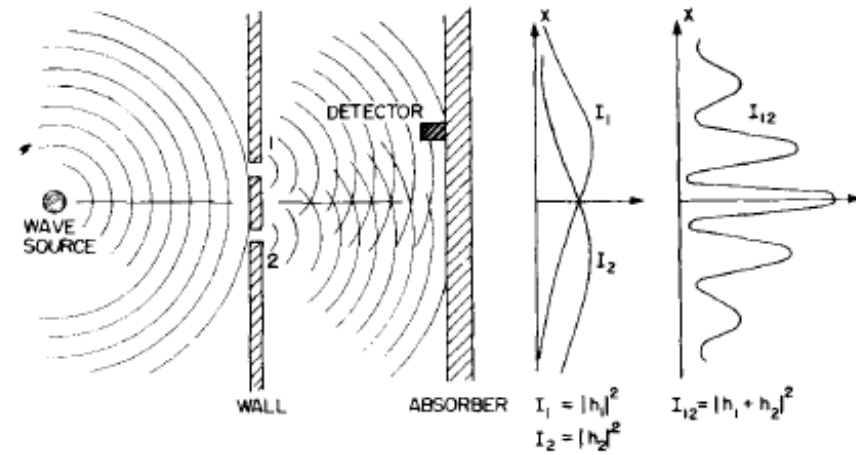
I_2 : intensity when hole 1 is closed.

I_{12} : intensity when both holes are open.

$$|h_1 + h_2|^2 = |h_1|^2 + |h_2|^2 + 2|h_1||h_2|\cos\delta,$$

$$I_{12} = I_1 + I_2 + 2\sqrt{I_1 I_2} \cos\delta.$$

Result: Constructive interference.



Contd.

Experiment with electrons:

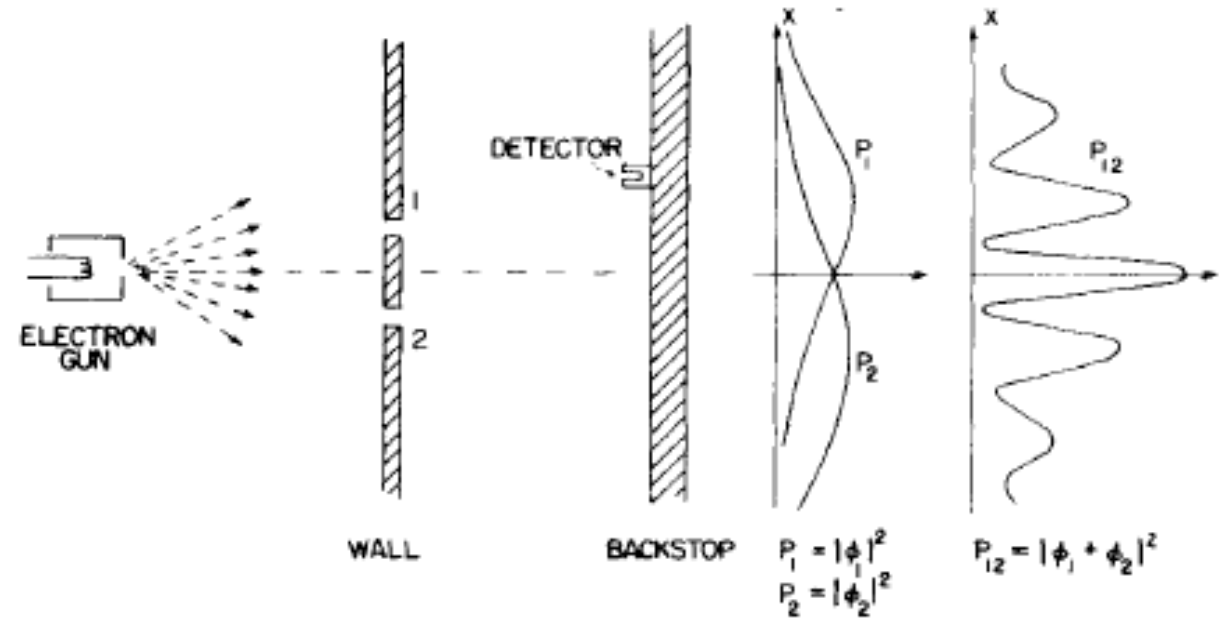
Detector records intensity of the wave.

P_1 : probability when hole 2 is closed.

P_2 : probability when hole 1 is closed.

P_{12} : probability when both holes are open.

Result: An interference !!!



$$P_{12} \neq P_1 + P_2.$$

Conclusion: the electrons arrive in lumps, like particles, and probability of arrival of these lumps is distributed like the distribution of the intensity of a wave. In this sense electrons behave like a particle and a wave.

Physical laws: classical point-of-view

Newtonian mechanics and Maxwell's theory of electromagnetism explain **macroscopic phenomena** but **fails** at **microscopic level**.

Laws of mechanics written in terms of **particle** trajectories. Here, **trajectory** implies path in **phase-space** defined in terms of **position** and **momentum** at all times i.e., $\{\mathbf{r}(t), \mathbf{p}(t); t \geq t_0\}$.

Classically, all properties of a particle (mass, position, momentum etc.) could be known to **infinite precision** (*in principle*, measuring instruments and experimental techniques can be perfected).

Knowing the **initial conditions** of a system, **Newton's laws predict the future – essence of determinism..**

So, what happens at microscopic level?

There are **no more particles** (in the classical sense) and associated **trajectories** at atomic level.

Classical theory fails badly at this level since the **“particle”** nature of the object under consideration itself **is not well defined**.

Particles at atomic level **exhibit wave-particle duality**.

A different perspective is needed to handle this strange wave-particle nature, something not encountered in **classical mechanics**, and which is

“Quantum Mechanics”

Quantum Mechanics

“Quantum mechanics is the description of the behavior of matter and light in all its details and, in particular, of the happenings on an atomic scale. Things on very small scale behaves like nothing that you have any direct experience about. They do not behave like waves, they do not behave like particles, they do not behave like clouds, or billiard balls, or weights on springs, or like anything that you have ever seen.”

R. P. Feynman

An **electron** is not a tiny planet orbiting around the nucleus. It is ***something*** which is **neither a particle nor a wave**.

Measured quantities in a physical theory are called **observables** (position, momentum etc.).

The **value** of these **observables** at any given time represents the **state** of the particle (or the system comprising of large number of particles).

contd.

Classically, a particle is in a **definite state**.

A **quantum state**, on the other hand, is a **superposition of all possible outcomes** of a measurement of physical properties.

Quantum mechanics is expressed in the language of probabilities.

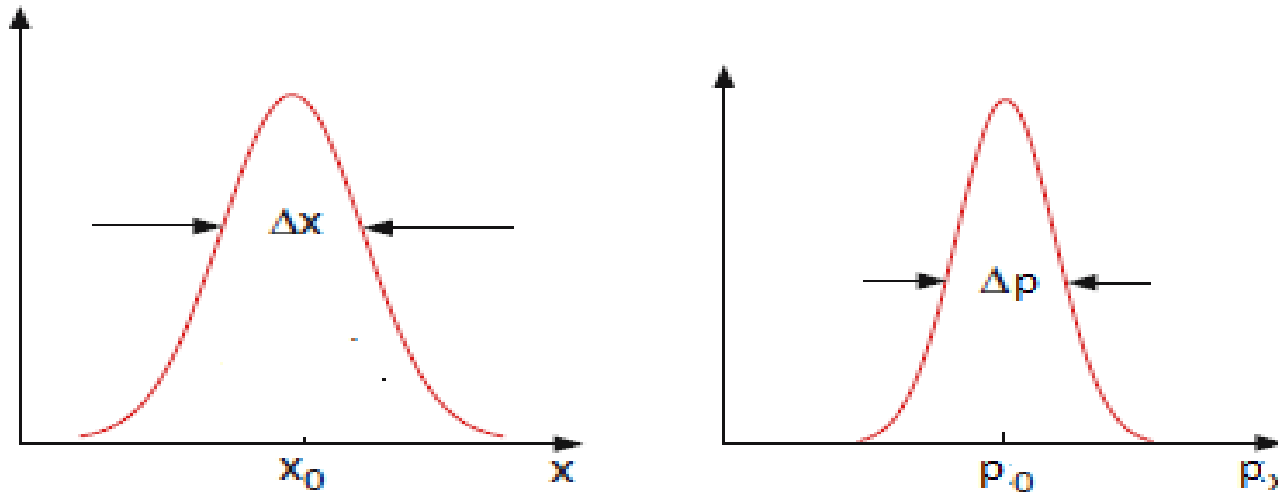
It is statistical in nature. Describes not a definite result of measurement on a system, rather, possible results of measurements on a large number of identical systems.

What is wrong with the trajectory at atomic level?

A set of measurement on the position (x) and momentum (p_x) in **a system of identical particles in a given state** (defines **an ensemble**) is in the form of a distribution.

Classically, errors in the measurement of x and p_x can be reduced to get the values x_0 and p_0 .

Quantum mechanically, such values cannot be assigned to a microscopic particle and is due to Uncertainty principle.



To be continued