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PEN205 MODERN PHYSICS

Quantum Mechanics – I

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quantum mechanics → an extremely successful theory for explaining the behavior of microscopic particles.

Contents:

The Wave Function

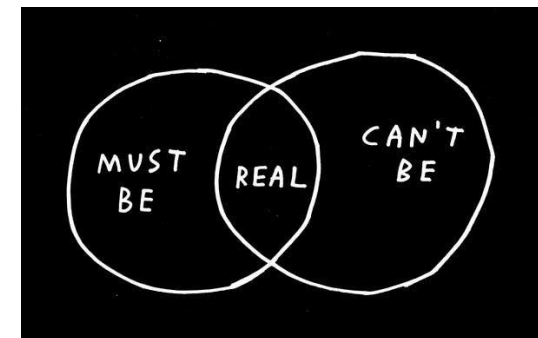
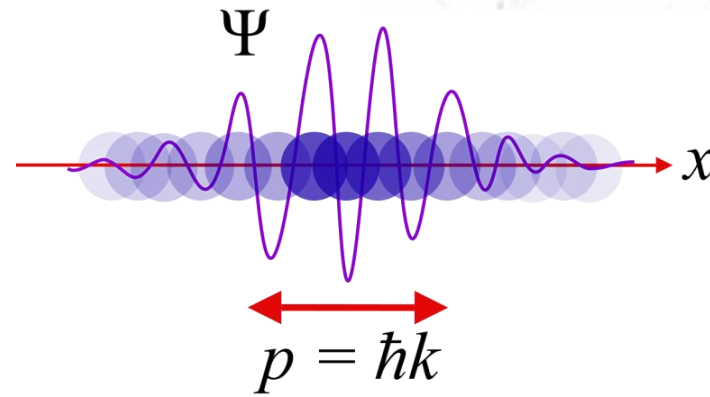
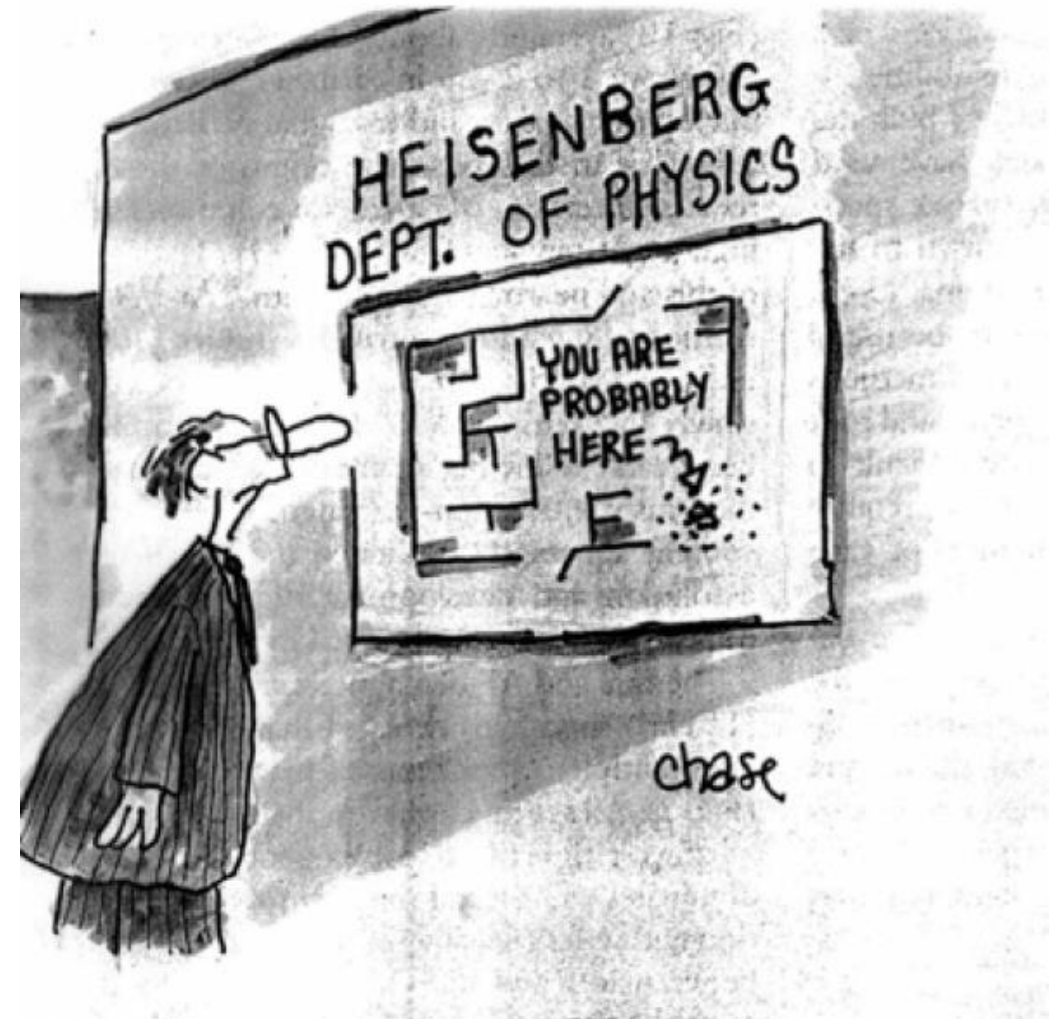
Quantum Particle Under Boundary Conditions

The Schrödinger Equation

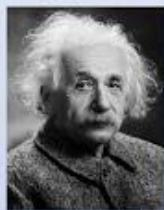
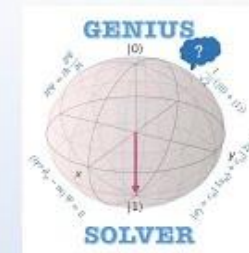
A Particle in a Well of Finite Height

Tunneling Through a Potential Energy Barrier

The Simple Harmonic Oscillator



Quantum Mechanics Timeline



Photoelectric effect
1905



Atomic Structure Model
1913



Introducing Spin
1924

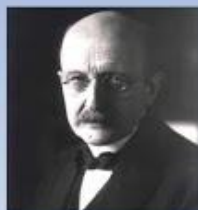


Solvay Conference
1927



Quantum Electrodynamics
1948 – 1950

1900
Black Body Radiation



1911
Discovery of Nucleus charge



1924
Wave-particle duality



1926
Non-relativistic QM



1927
Uncertainty Principle



1928
Relativistic QM

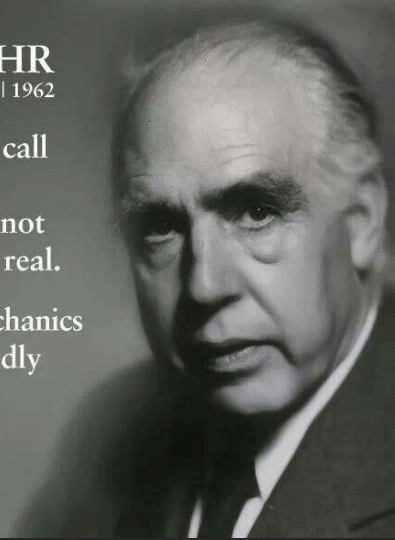


NIELS BOHR

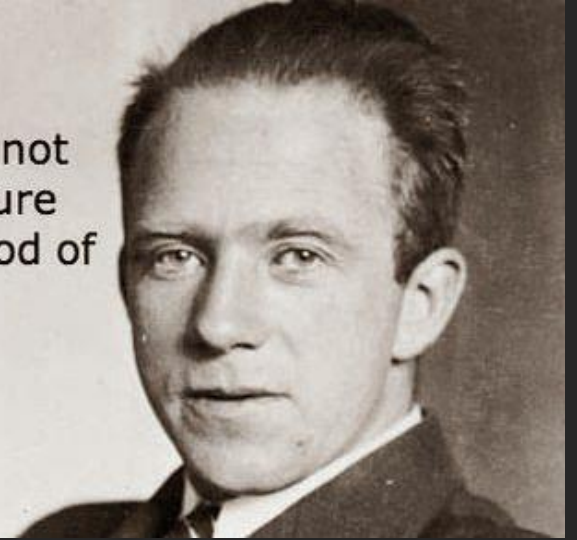
7 | 10 | 1885 – 18 | 11 | 1962

Everything we call
real is made of
things that cannot
be regarded as real.

If quantum mechanics
hasn't profoundly
shocked you,
you haven't
understood
it yet.

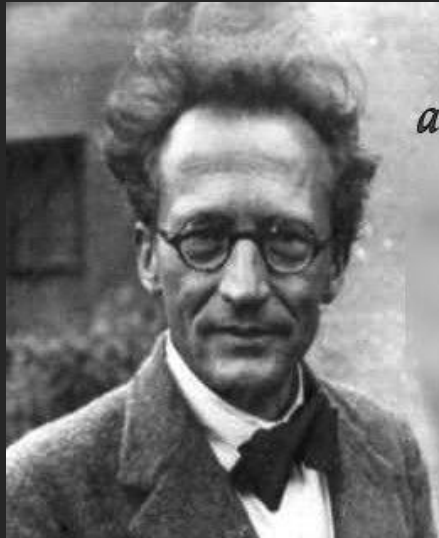


"What we observe is not
nature itself, but nature
exposed to our method of
questioning."
-Werner Heisenberg



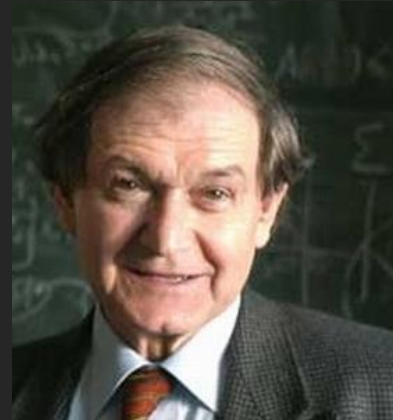
*What we observe
as material bodies and forces
are nothing but shapes
and variations
in the structure of space*

ERWIN SCHRÖDINGER



Quantum mechanics makes
absolutely no sense.

— *Roger Penrose* —

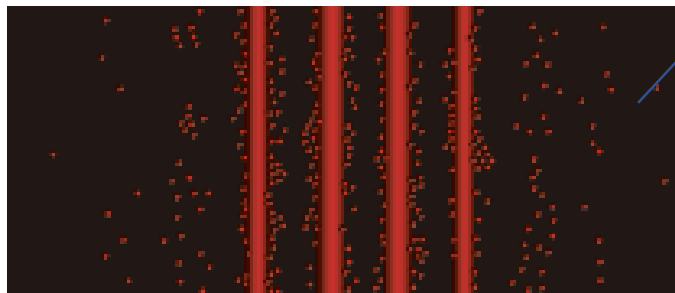
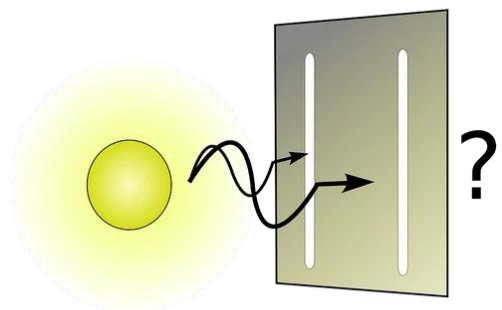


The Wave Function

from previous lesson → both matter and electromagnetic radiation are sometimes best modeled as particles and sometimes as waves, depending on the phenomenon being observed.

We can improve our understanding of quantum physics by making another connection between particles and waves using the notion of **probability**

Let's remember Double Slit Experiment;



the electrons are detected as particles at a localized spot on the detector screen at some instant of time, but the **probability** of arrival at that spot is determined by finding the intensity of two interfering waves.

If particles are waves, what's waving?

→ **Probability**

Uncertainty Principle

Classical mechanics specifies everything in the system in a fully deterministic way



In QM → it is fundamentally impossible to make simultaneous measurements of a particle's position and momentum with infinite accuracy.

The uncertainty principle arises from the **wave-particle duality**;

- ✓ Every particle has a wave associated with it and each particle exhibits wavelike behavior. $\lambda = h/p$
- ✓ The particle is most likely to be found in those places where the undulations of the wave are greatest, or most intense.
- ✓ The more intense the undulations of the associated wave become, however, the more ill-defined becomes the wavelength, which in turn determines the momentum of the particle.

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

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

The uncertainty principle states that the more precisely the position of some particle is determined, the less precisely its momentum can be predicted from initial conditions, and vice versa.

Let's begin by discussing electromagnetic radiation using the **particle model**

- The probability per unit volume of finding a **photon** in a given region of space at an instant of time is proportional to the number of photons per unit volume at that time;
- The number of photons per unit volume is proportional to the intensity of the radiation;
- intensity of electromagnetic radiation is proportional to the square of the electric field amplitude E for the electromagnetic wave;

$$\frac{\text{Probability}}{V} \propto \frac{N}{V}$$

$$\frac{N}{V} \propto I$$

$$I \propto E^2$$

By combining these equations, we can form a connection between the particle model and the wave model;

$$\frac{\text{Probability}}{V} \propto E^2$$

Therefore, for electromagnetic radiation, the probability per unit volume of finding a particle associated with this radiation (the photon) is proportional to the square of the amplitude of the associated electromagnetic wave.

Is there a parallel proportionality for a material particle?

Is the probability per unit volume of finding the **particle** proportional to the square of the amplitude of a wave representing the particle?

From previous lesson → we learned that **de Broglie** wave associated with every particle

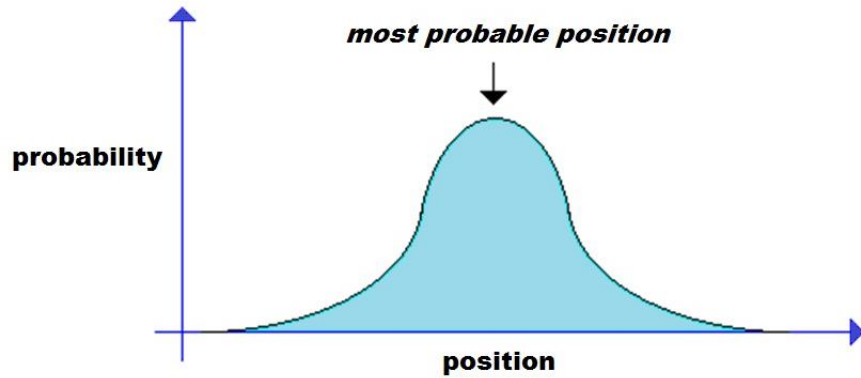
- The amplitude of the de Broglie wave associated with a particle is not a measurable quantity because the wave function representing a particle is generally a complex function.
- In contrast, the electric field for an electromagnetic wave is a real function.

$$\frac{\text{Probability}}{V} \propto E^2$$

→ So, matter analogue of this equation relates to the square of the amplitude of the wave to the probability per unit volume of finding the particle

Hence, the amplitude of the wave associated with the particle is called the **probability amplitude**, or the **wave function**, and it has the symbol Ψ

Quantum Wave Function



In general, the complete wave function Ψ for a system depends on the positions of all the particles in the system and on time;

$$\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_j, \dots, t)$$

\vec{r}_j is the position vector of the j^{th} particle in the system.

the wave function Ψ is mathematically separable in space and time;

$$\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_j, \dots, t) = \psi(\vec{r}_j) e^{-i\omega t}$$

The wave function contains within it all the information that can be known about the particle

$$\underbrace{\omega (= 2\pi f) \quad i = \sqrt{-1}}_{\text{angular frequency of the wave function}}$$

The wave function Ψ is often complex-valued \rightarrow The absolute square $|Y(x)|^2$ is always real and positive and is proportional to the probability per unit volume of finding a particle at a given point at some instant.

reminder:

²For a complex number $z = a + ib$, the complex conjugate is found by changing i to $-i$: $z^* = a - ib$. The product of a complex number and its complex conjugate is always real and positive. That is, $z^*z = (a - ib)(a + ib) = a^2 - (ib)^2 = a^2 - (i)^2b^2 = a^2 + b^2$.

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

ψ^* : complex conjugate of ψ

Probability Density

If dV is a small volume element surrounding some point, the probability of finding the particle in that volume element is ;

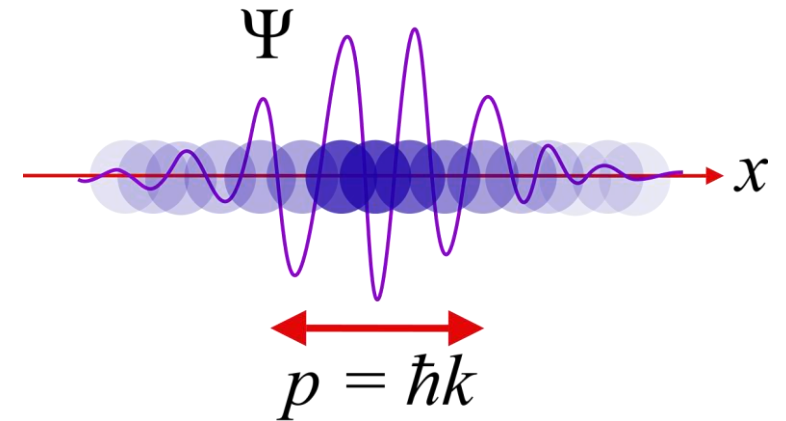
This probabilistic interpretation of the wave function was first suggested by Max Born in 1928.

$$P(x, y, z) dV = |\psi|^2 dV$$

The wave function Ψ for an ideal free particle moving along the x axis can be written as

$$\psi(x) = Ae^{ikx}$$

constant amplitude ← A → $k = 2\pi/\lambda$, the angular wave number



Probability in one dimension \rightarrow

$$P(x) dx = |\psi|^2 dx$$

it is not possible to specify the position of a particle with complete certainty, but it is possible through $|\psi(x)|^2$ to specify the probability of observing it in a region surrounding a given point x ;

So, the probability of the particle being between a and b is given by:

$$P_{ab} = \int_a^b |\psi|^2 dx$$

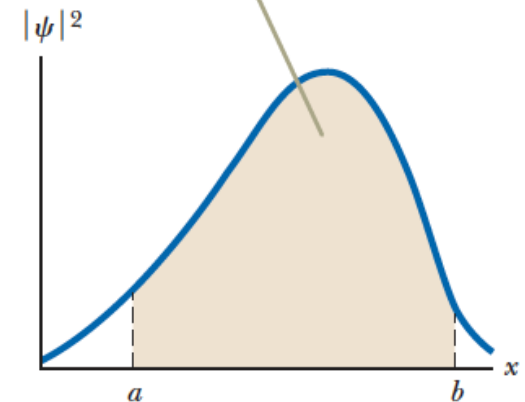
The value of that probability must lie between the limits 0 and 1.

For example, if the probability is 0.30, there is a 30% chance of finding the particle in the interval.

Because the particle must be somewhere along the x axis, the sum of the probabilities over all values of x must be 1:

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

The probability of a particle being in the interval $a \leq x \leq b$ is the area under the probability density curve from a to b .



Any wave function satisfying this equation is said to be **normalized**.

Once the wave function for a particle is known, it is possible to calculate the average position at which you would expect to find the particle after many measurements. This average position is called the **expectation value** of x

$$\langle x \rangle \equiv \int_{-\infty}^{\infty} \psi^* x \psi dx$$

Example: Consider a particle whose wave function is given by $\psi(x) = Ae^{-ax^2}$

(A) What is the value of A if this wave function is normalized?

Let's apply the normalization condition

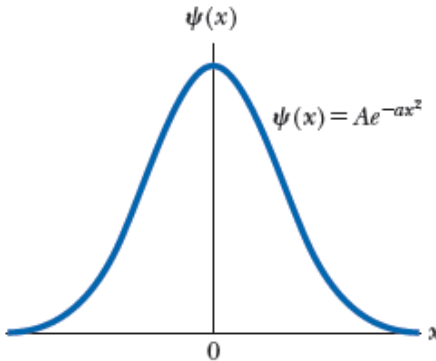
$$\int_{-\infty}^{\infty} |\psi|^2 dx = \int_{-\infty}^{\infty} (Ae^{-ax^2})^2 dx = A^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = 1$$

$$\int_0^{\infty} e^{-2ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{2a}}$$

$$2A^2 \left(\frac{1}{2} \sqrt{\frac{\pi}{2a}} \right) = 1 \rightarrow A = \left(\frac{2a}{\pi} \right)^{1/4}$$

(B) What is the expectation value of x for this particle?

$$\begin{aligned} \langle x \rangle &\equiv \int_{-\infty}^{\infty} \psi^* x \psi dx = \int_{-\infty}^{\infty} (Ae^{-ax^2}) x (Ae^{-ax^2}) dx \\ &= A^2 \int_{-\infty}^{\infty} x e^{-2ax^2} dx \\ &= 0 \end{aligned}$$



it is not surprising that the average position of the particle is 0, due to the symmetry of wave function