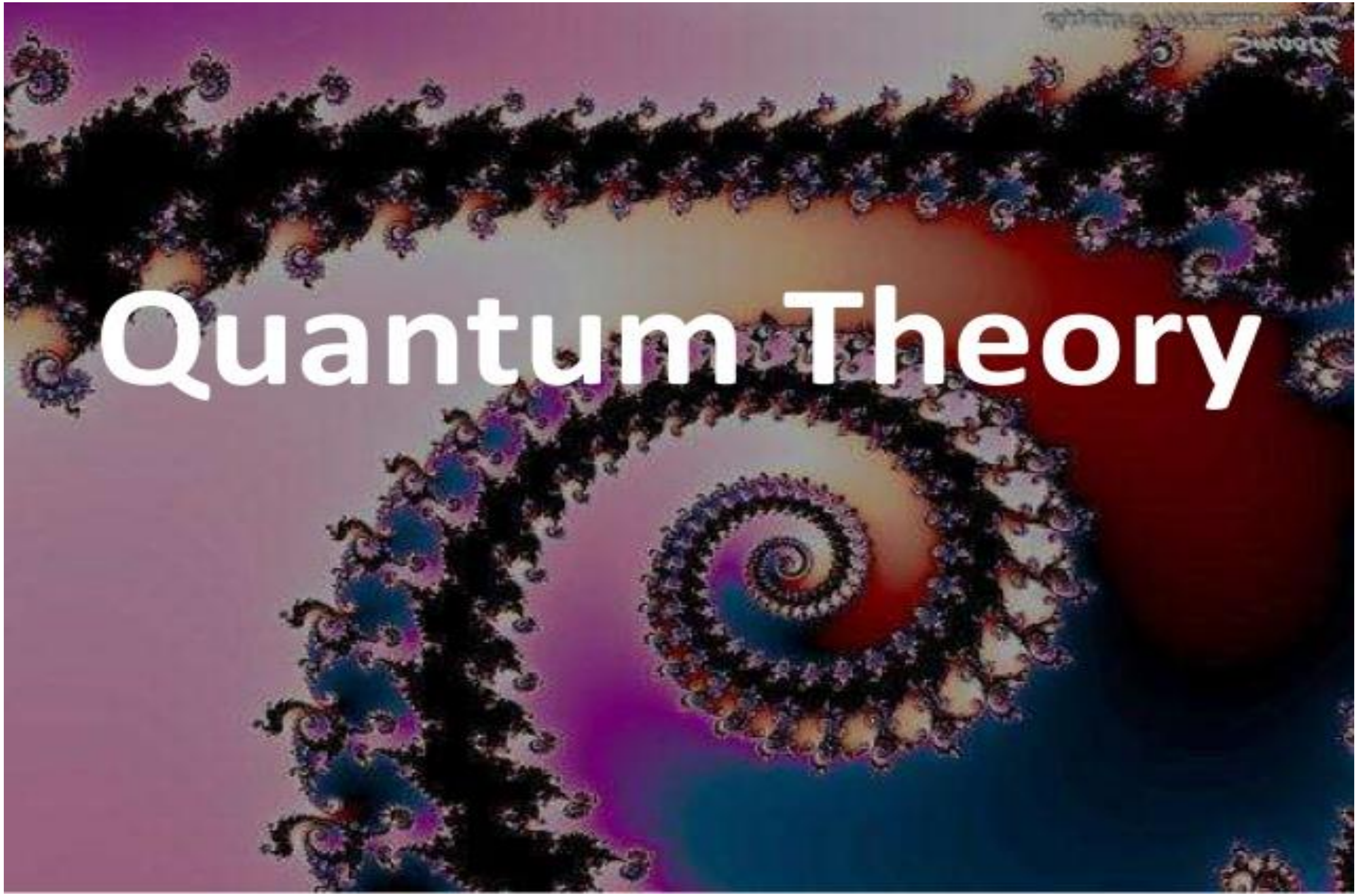

Quantum Theory

Quantum Theory is a theory about dead cats.

More seriously, it is a description of the way the small particles that make up the universe behave.

Their behaviour is quite different from the behaviour of the larger objects with which we are familiar from everyday life.

Thus quantum theory can seem quite counter-intuitive.

Quantum theory (or quantum mechanics) was developed mostly between 1900 and 1930
by European physicists including

Max Planck
Albert Einstein
Neils Bohr
Louis de Broglie
Max Born
Paul Dirac
Werner Heisenberg
Wolfgang Pauli
Erwin Schrodinger and his cat
Richard Feynman

As well as quantum theory,
these 30 years brought the discovery of relativity,
galaxies beyond the Milky Way,
and the expanding universe.

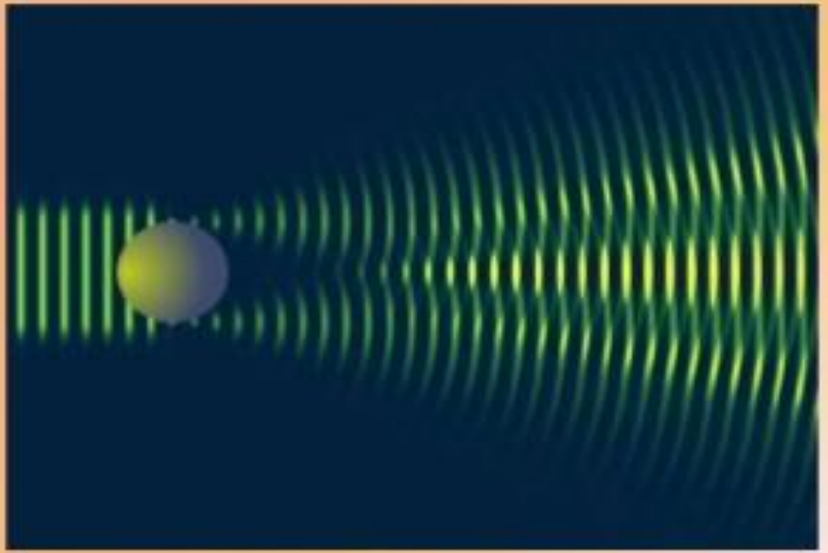
These discoveries laid the foundations of modern physics and cosmology.

In the 17th Century Newton came up with a theory of light.

He said that light is made of particles, each particle consisting of a particular colour of the spectrum.

This was just after coming up with his laws of motion and gravitation and developing calculus.

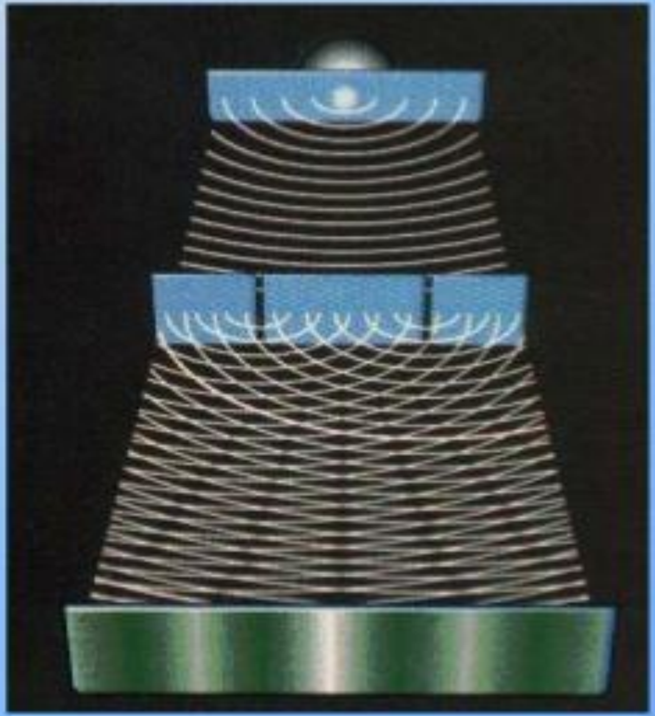
During the 18th Century, most scientists accepted this, though a few, like Robert Hooke, Christian Huygens and Leonhard Euler believed that light consisted of waves rather than particles.



Then in 1803, Thomas Young did his famous double-slit experiment.

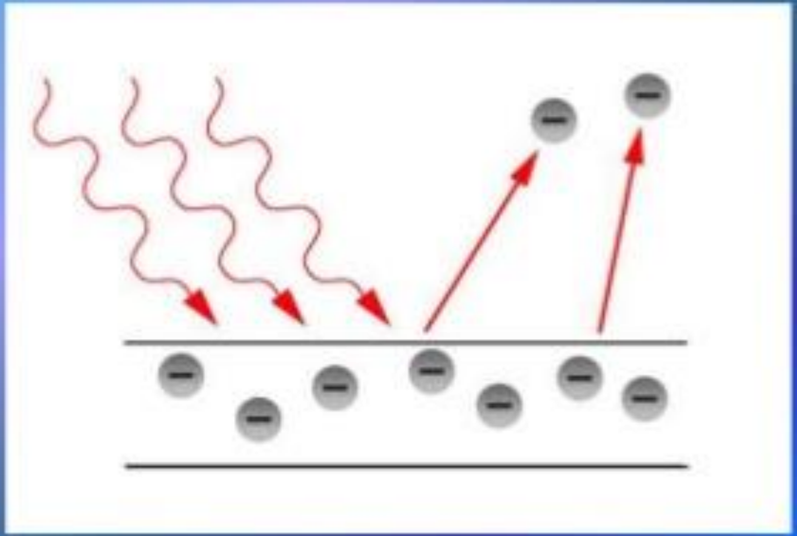
The interference Patterns produced were the same as those produced by waves on water.

After this it was generally accepted that light was made of waves rather than particles.



However, in 1905, Einstein produced a paper on the photo-electric effect, showing that light really was made of particles.

Light was used to provide the energy to dislodge electrons from a metal.



A certain amount of energy was required to dislodge an electron.

It was expected that once the brightness of the light reached a certain level, electrons would be released.

What he found, though, was that the brightness made no difference – what mattered was the colour.
Very dim blue light would release electrons while very bright red light would not.

It seemed that light was made up of particles of different colour, just as Newton had suggested. Einstein called them photons.

Bluer colours has shorter wavelengths and therefore higher frequencies and higher energies.

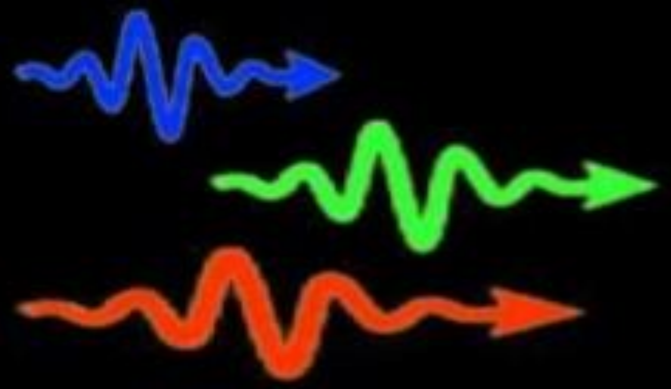
The energy of a photon was proportional to the frequency

$$E = hf$$

the constant of proportionality being called Planck's constant and having the value 6.6×10^{-34}.

A red photon did not have enough energy to dislodge an electron and no intensity of red light would do the job.

However, a single blue photon did have enough energy.

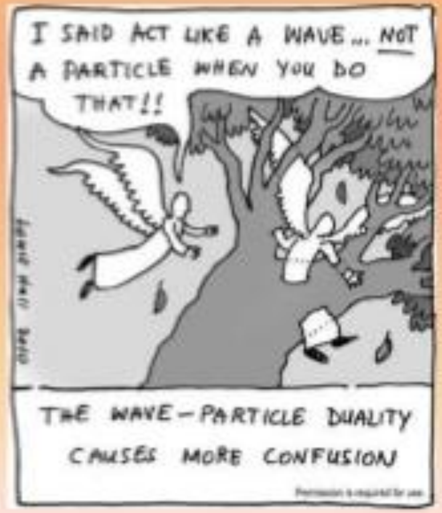


This showed that the energy of light came in discrete packets called quanta (plural of quantum).

Each quantum consisted of a fixed amount of energy.

So now it seemed that light was both a wave and a particle. Eddington suggested calling it a wavicle, though this idea didn't really stick.

It is now well accepted that photons behave in some ways as waves and in other ways as particles.



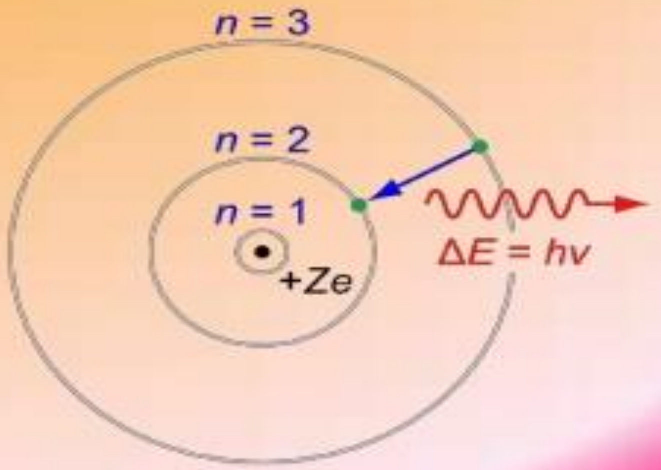
This was not actually the start of quantum theory. It started 5 years earlier in 1900 when Max Planck published a paper showing that black body radiation was quantized.

The idea behind this is harder to understand though.

In 1913, Niels Bohr came up with a model of the hydrogen atom which explained experimental observations.

In his model, electrons could orbit the nucleus only at certain distances.

When energy was absorbed or emitted, it did so only in quantities equal to the difference between the energy levels of the orbits.



Thus a hydrogen emitted light only at certain discrete frequencies.

Introduction

There are a few phenomenon which the classical mechanics failed to explain.

1. Stability of an atom
2. Spectral series of Hydrogen atom
3. Black body radiation

Max Planck in 1900 at a meeting of German Physical Society read his paper "On the theory of the Energy distribution law of the Normal Spectrum". This was the start of the revolution of Physics i.e. the start of **Quantum Mechanics.**

It is a generalization of Classical Physics that includes classical laws as special cases.

Quantum Physics extends that range to the region of small dimensions.

Just as ‘c’ the velocity of light signifies universal constant, the Planck's constant characterizes Quantum Physics.

$$h = 6.65 \times 10^{-27}\, erg.\mathrm{sec}$$

$$h = 6.625 \times 10^{-34}\, Joule.\mathrm{sec}$$

Quantum Mechanics

It is a generalization of Classical Physics that includes classical laws as special cases.

Quantum Physics extends that range to the region of small dimensions.

Just as ‘c’ the velocity of light signifies universal constant, the Planck's constant characterizes Quantum Physics.

$$h = 6.65 \times 10^{-27}\, erg.\mathrm{sec}$$

$$h = 6.625 \times 10^{-34}\, Joule.\mathrm{sec}$$

Quantum Mechanics

It is able to explain

1. Photo electric effect
2. Black body radiation
3. Compton effect
4. Emission of line spectra

The most outstanding development in modern science was the conception of Quantum Mechanics in 1925. This new approach was highly successful in explaining about the behavior of atoms, molecules and nuclei.

Wave Particle Duality

Light can exhibit both kind of nature of waves and particles so the light shows wave-particle dual nature.

In some cases like interference, diffraction and polarization it behaves as wave while in other cases like photoelectric and compton effect it behaves as particles (photon).

De Broglie Waves

Not only the light but every materialistic particle such as electron, proton or even the heavier object exhibits wave-particle dual nature.

De-Broglie proposed that a moving particle, whatever its nature, has waves associated with it. These waves are called “**matter waves**”.

Energy of a photon is

$$E = h\nu$$

For a particle, say photon of mass, m

$$E = mc^2$$

$$mc^2 = h\nu$$

$$mc^2 = \frac{hc}{\lambda}$$

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

Suppose a particle of mass, m is moving with velocity, v then the wavelength associated with it can be given by

$$\lambda = \frac{h}{mv} \quad \text{or} \quad \lambda = \frac{h}{p}$$

(i) If $v = 0 \Rightarrow \lambda = \infty$ means that waves are associated with **moving** material particles only.

(ii) De-Broglie wave does not depend on whether the moving particle is charged or uncharged. It means matter waves are not electromagnetic in nature.

Heisenberg Uncertainty Principle

It states that only one of the “position” or “momentum” can be measured accurately at a single moment within the instrumental limit.

or

It is impossible to measure both the position and momentum simultaneously with unlimited accuracy.

$\Delta x \rightarrow$ uncertainty in position

$\Delta p_x \rightarrow$ uncertainty in momentum

then $$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$ $$\therefore \hbar = \frac{h}{2\pi}$$

The product of Δx & Δp_x of an object is greater than or equal to $\frac{\hbar}{2}$

If Δx is measured accurately i.e. $\Delta x \to 0 \quad \Rightarrow \Delta p_x \to \infty$

The principle applies to all canonically conjugate pairs of quantities in which measurement of one quantity affects the capacity to measure the other.

Like, energy E and time t.

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

and angular momentum L and angular position θ

$$\Delta L \Delta \theta \geq \frac{\hbar}{2}$$

Schrodinger: A Wave Equation for Electrons

$$E = \hbar\omega \qquad\qquad p = \hbar k$$

Schrodinger ***guessed*** that there was some wave-like quantity that could be related to energy and momentum …

$$\psi \approx e^{j(\omega t - k_x x)}$$ wavefunction

$$\frac{\partial}{\partial t}\psi = j\omega\psi \quad \Rightarrow \quad E\psi = \hbar\omega\psi = -j\hbar\frac{\partial}{\partial t}\psi$$

$$\frac{\partial}{\partial x}\psi = -jk_x\psi \quad \Rightarrow \quad p_x\psi = \hbar k_x\psi = j\hbar\frac{\partial}{\partial x}\psi$$

Schrodinger: A Wave Equation for Electrons

$$E\psi = \hbar\omega\psi = -j\hbar\frac{\partial}{\partial t}\psi \qquad p_x\psi = \hbar k\psi = j\hbar\frac{\partial}{\partial x}\psi$$

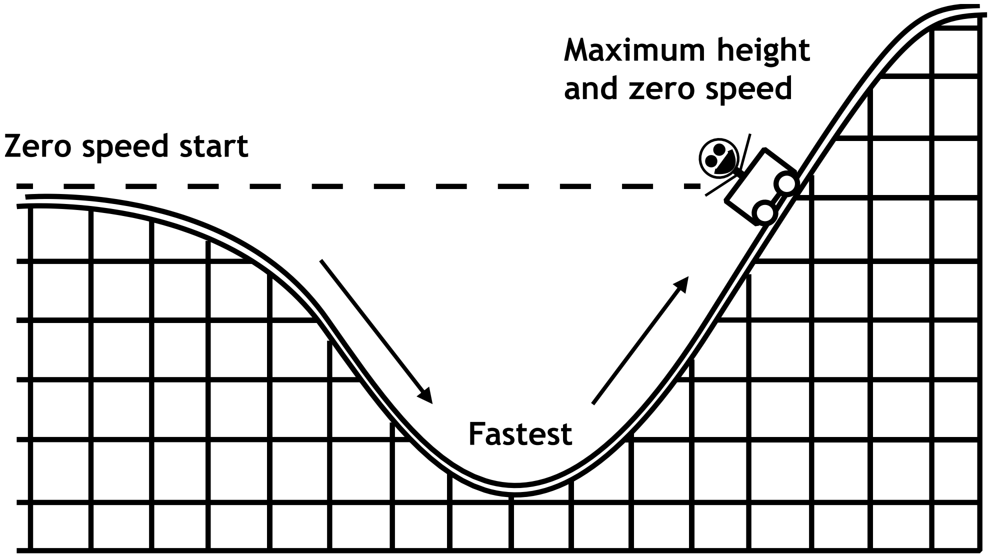
$$E = \frac{p^2}{2m}$$ (free-particle)

$$\boxed{-j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}}$$ (free-particle)

..The Free-Particle Schrodinger Wave Equation !

Erwin Schrödinger (1887–1961)
Image in the Public Domain

Classical Energy Conservation



- total energy = kinetic energy + potential energy
- In classical mechanics, $E = K + V$
- *V* depends on the system
  - e.g., gravitational potential energy, electric potential energy

Schrodinger Equation and Energy Conservation

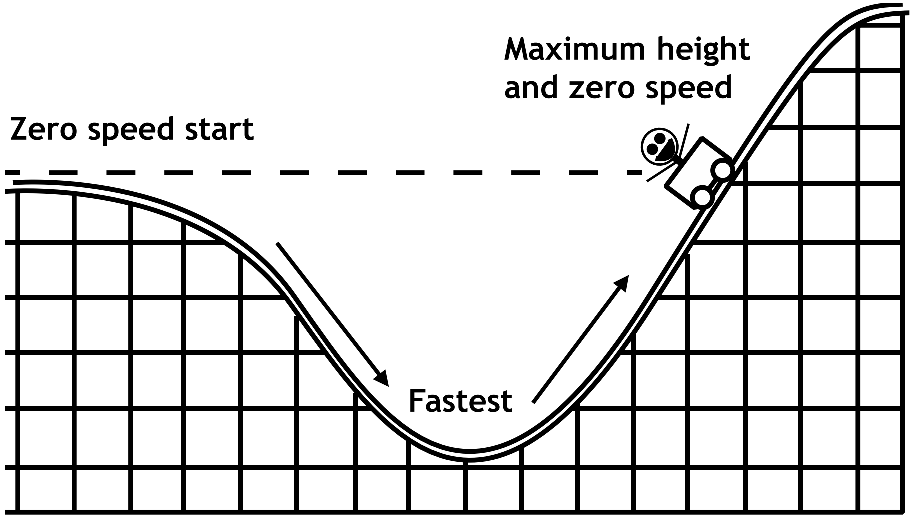
... The Schrodinger Wave Equation !

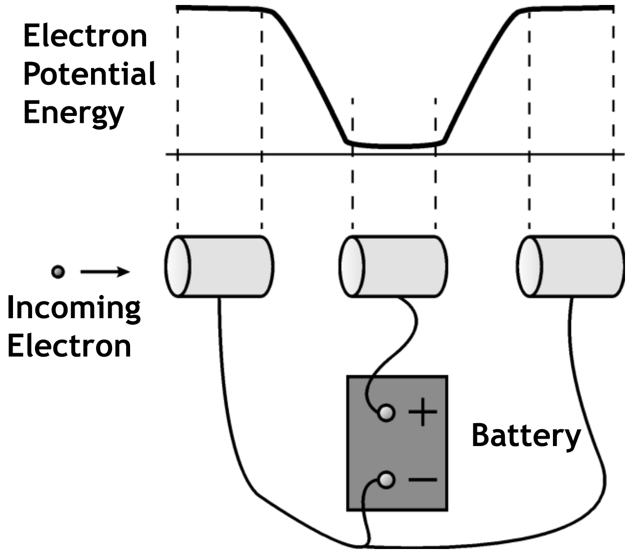
$$E = K + V \quad \Longrightarrow \quad \boxed{-j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi}$$

Total E term **K.E. term** **P.E. term**

... In physics notation and in 3-D this is how it looks:

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





Time-Dependent Schrodinger Wave Equation

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

PHYSICS NOTATION

Total E term

K.E. term

P.E. term

$$\Psi(x,t) = e^{-iEt/\hbar}\psi(x)$$

Time-Independent Schrodinger Wave Equation

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

Electronic Wavefunctions

$$\psi(x) \approx e^{j(\omega t - k_x x)}$$ free-particle wavefunction

- Completely describes all the properties of a given particle
- Called $\psi = \psi$ (x,t) - is a complex function of position x and time t
- What is the meaning of this wave function?

  - The quantity $|\psi|^2$ is interpreted as the probability that the particle can be found at a particular point x and a particular time t

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

Image is in the public domain

Werner Heisenberg (1901–1976)
Image in the Public Domain

Copenhagen Interpretation of Quantum Mechanics

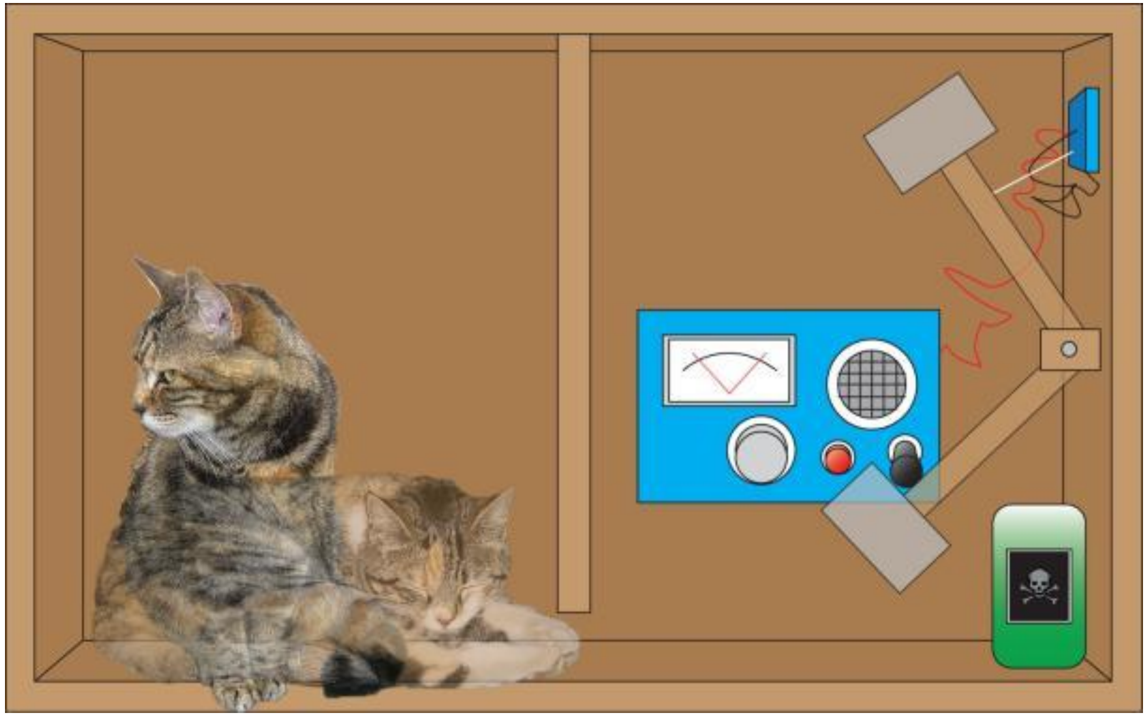
- A system is completely described by a wave function ψ, representing an observer's subjective knowledge of the system.
- The description of nature is essentially probabilistic, with the probability of an event related to the square of the amplitude of the wave function related to it.
- It is not possible to know the value of all the properties of the system at the same time; those properties that are not known with precision must be described by probabilities. (Heisenberg's uncertainty principle)
- Matter exhibits a wave–particle duality. An experiment can show the particle-like properties of matter, or the wave-like properties; in some experiments both of these complementary viewpoints must be invoked to explain the results.
- Measuring devices are essentially classical devices, and measure only classical properties such as position and momentum.
- The quantum mechanical description of large systems will closely approximate the classical description.

day’s Culture Moment

Schrödinger's cat

“It is typical of these cases that an indeterminacy originally restricted to the atomic domain becomes transformed into macroscopic indeterminacy, which can then be resolved by direct observation. That prevents us from so naively accepting as valid a "blurred model" for representing reality. In itself, it would not embody anything unclear or contradictory. There is a difference between a shaky or out-of-focus photograph and a snapshot of clouds and fog banks.”

-Erwin Schrodinger, 1935



SCHRÖDINGER'S CAT IS DEAD

Comparing EM Waves and Wavefunctions

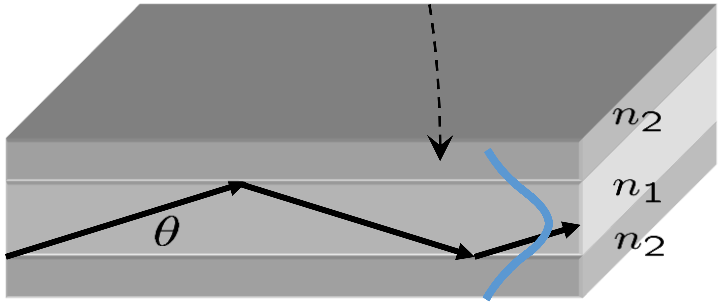
EM WAVES

$$\omega^2 = c^2 k^2$$

$$-\frac{\partial^2}{\partial t^2}\vec{E} = -c\frac{\partial^2}{\partial x^2}\vec{E}$$

$$I = \frac{|E|^2}{\eta}$$

waveguide



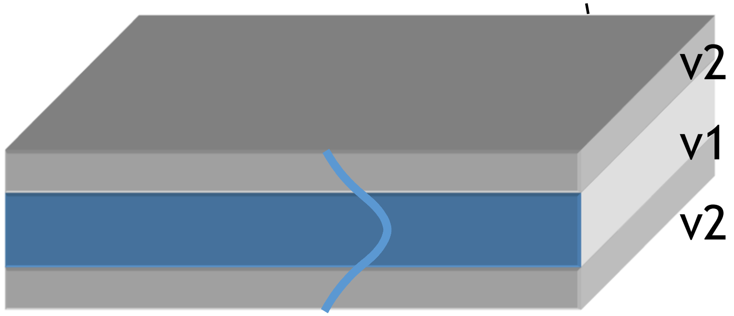
QM WAVEFUNCTIONS

$$E = \frac{p^2}{2m} + V(x)$$

$$-j\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

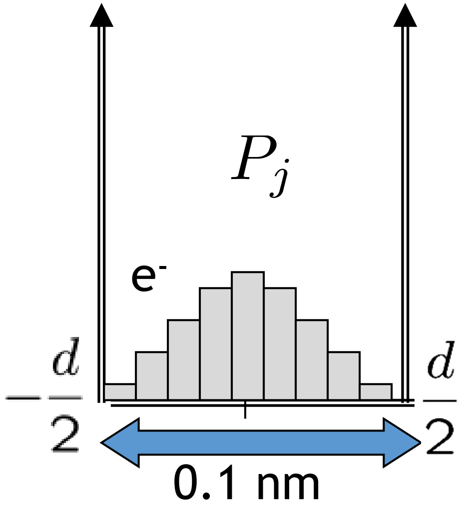
$$P(x)dx = |\psi|^2$$

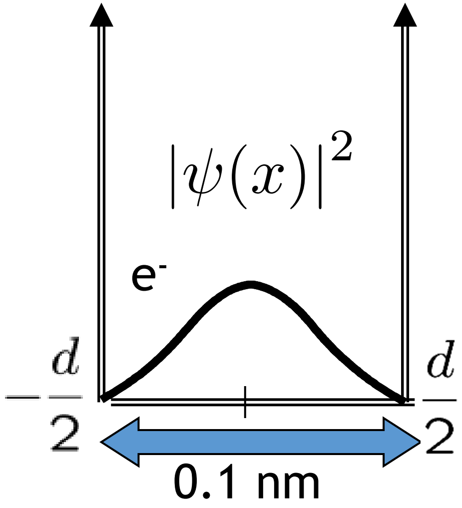
Quantum well



Expected Position

$$\langle x \rangle = \sum_{j=-\infty}^{\infty} x\, P_j \qquad \langle x \rangle = \int_{-\infty}^{\infty} x|\psi|^2 dx$$





$$< x >= 0 \qquad < x >= 0$$

Expected Momentum

$$< p >= \int_{-\infty}^{\infty} p \left|\psi(x)\right|^2 dx$$

$$= \int_{-\infty}^{\infty} j\hbar \frac{\partial}{\partial x} \left|\psi(x)\right|^2 dx$$

imaginary

real

Doesn't work !
Need to guarantee <p> is real

… so let's fix it by rewriting the expectation value of p as:

$$< p >= \int_{-\infty}^{\infty} \psi^*(x) \left(j\hbar \frac{\partial}{\partial x} \right) \psi(x) dx$$

free-particle wavefunction

$$\psi \approx e^{j(\omega t - k_x x)} \qquad < p >= \hbar k$$

Maxwell and Schrodinger

Maxwell's Equations

$$\oint_C \vec{E} \cdot d\vec{l} = -\frac{d}{dt}\left(\int_S \vec{B} \cdot d\vec{l}\right)$$

$$\oint_C \vec{H} \cdot d\vec{l} = \int \vec{J} \cdot d\vec{A} + \frac{d}{dt}\int_S \epsilon\vec{E} \cdot d\vec{A}$$

The Wave Equation

$$\frac{\partial^2 E_y}{\partial z^2} = \epsilon\mu\frac{\partial^2 E_y}{\partial t^2}$$

Dispersion Relation

$$\omega^2 = c^2 k^2$$

$$\omega = ck$$

Energy-Momentum

$$E = \hbar\omega = \hbar ck = cp$$

Quantum Field Theory

The Schrodinger Equation

$$-j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$$

(free-particle)

Dispersion Relation

$$\hbar\omega = \frac{\hbar^2 k^2}{2m}$$

Energy-Momentum

$$E = \frac{p^2}{2m}$$ (free-particle)