



# Quantum Mechanics

for Computing Apps

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Francisco Treviño

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Continental México

1. On the shoulders of giants...
2. Framework
3. Particle aspect of radiation
4. Wave Aspect of Particles
5. Particles vs Waves
6. Computational Quantum Mechanics

## Quantum

- The amount or quantity observably present, or available. [18th c.]
- (physics) The smallest possible, and therefore indivisible, unit of a given quantity or quantifiable phenomenon. [20th c.]
- (computing) The amount of time allocated for a thread to perform its work in a multithreaded environment.

**On the shoulders of giants...**

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# Copenhagen interpretation



**Figure 1:** Solvay Conference 1927 (17/29 Nobel prizes)

# Framework

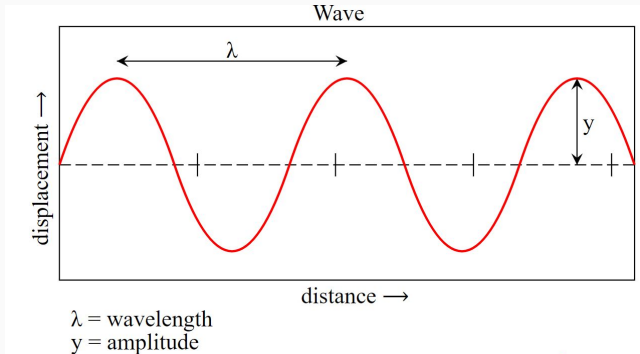
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Relativistic Energy:  $E = mc^2$

Momentum:  $p = mv$

Radiation: transmission of energy through space.

# Waves

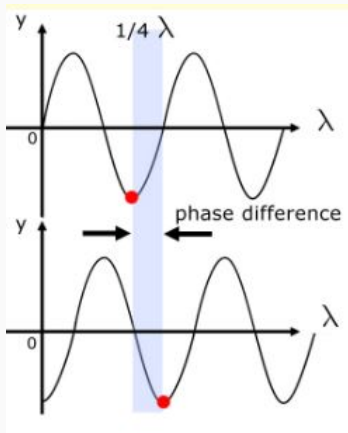


Frequency:  $\nu = \frac{c}{\lambda}$

Electromagnetic Waves transport energy and momentum.

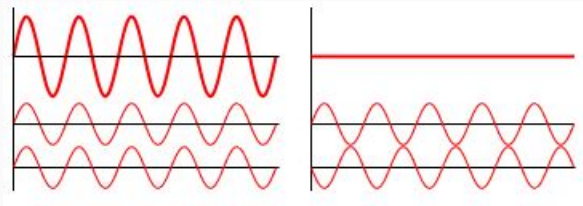


# Waves: phase



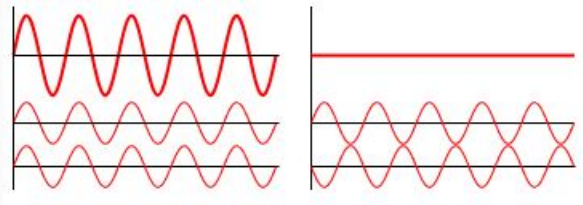
**Figure 2:** Wave phase

# Waves: Interference



**Figure 3:** Waves interference

# Waves: Interference



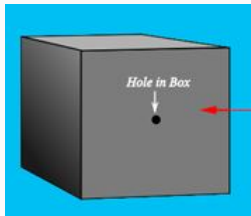
**Figure 3:** Waves interference

LASER: wave sources are perfectly **coherent** if they have a constant phase difference and the same frequency, and the same waveform.

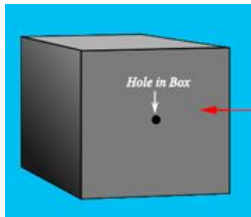
# Particle aspect of radiation

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# Blackbody radiation [1900]



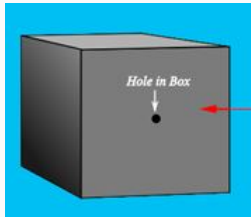
# Blackbody radiation [1900]



Planck's quantization rule: the energy exchange between radiation and matter *must be discrete*:

$$E = nh\nu, \quad n = 1, 2, 3, \dots$$

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$h\nu$  is the energy of a "quantum" of radiation,  $\nu$  represents the frequency of an oscillating charge.

# Particle behavior of Waves

- Planck's new idea, the *discrete* exchange of energy, solved the “ultraviolet catastrophe” as it matches experimental data.
- The spectrum of the blackbody radiation reveals the quantization of radiation, notably the particle behavior of electromagnetic waves.



# The end of the world as we know it...

The introduction of the constant  $h$  had indeed heralded the *end of classical physics* and the dawn of a new era: physics of the microphysical world.

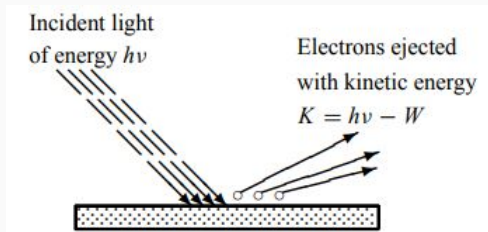
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$$h = 6.62 \times 10^{-34} \text{ J} \cdot \text{s}$$

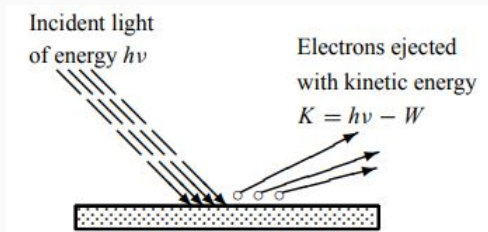
For a mass of 1 kg, length of 1 m, time 1 s, the Action =  $981 \times 10^2 \text{ J} \cdot \text{s}$

# Photoelectric Effect [1905]



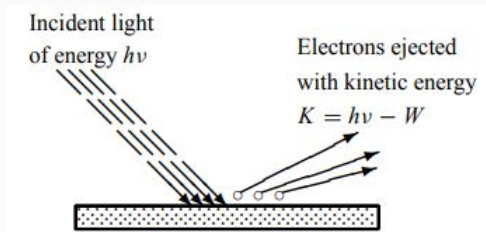
Einstein assumed that light is made of corpuscles each carrying an energy  $h\nu$ , called *photons*.

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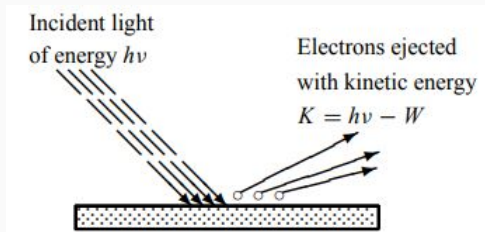
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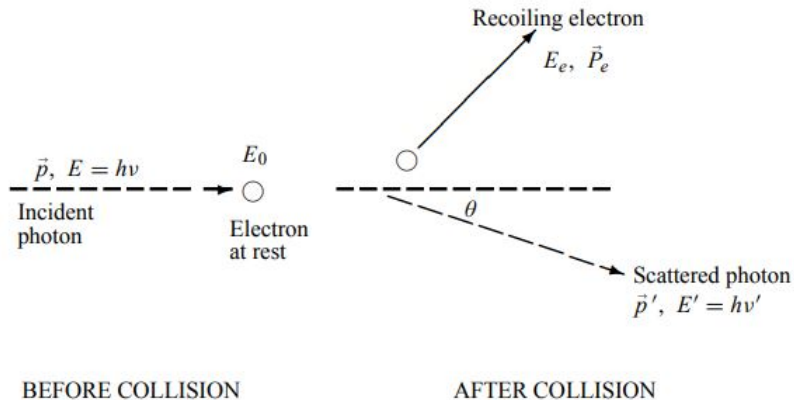


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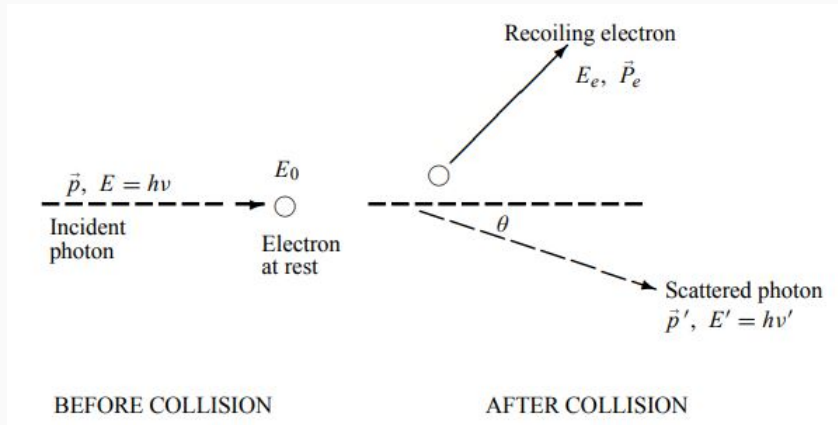
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Photoelectric effect does provide compelling evidence for the corpuscular nature of the electromagnetic radiation.

# Compton Effect [1923]



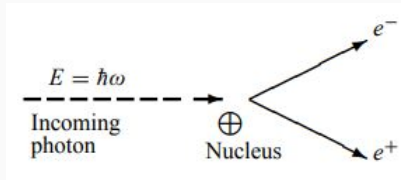
# Compton Effect [1923]



Compton effect confirms that photons behave like particles: they collide with electrons like material particles

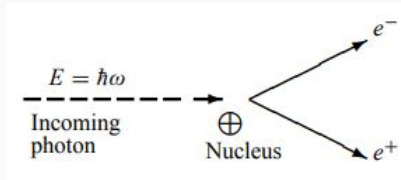


# Pair production, annihilation [1932]



- Predicted by Dirac's relativistic quantum mechanics
- Is a direct consequence of the mass-energy equation of Einstein  $E = mc^2$  which states that pure energy can be converted into mass and vice versa

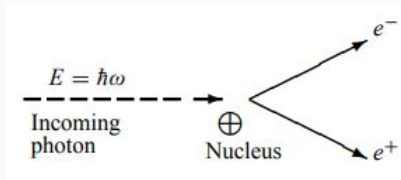
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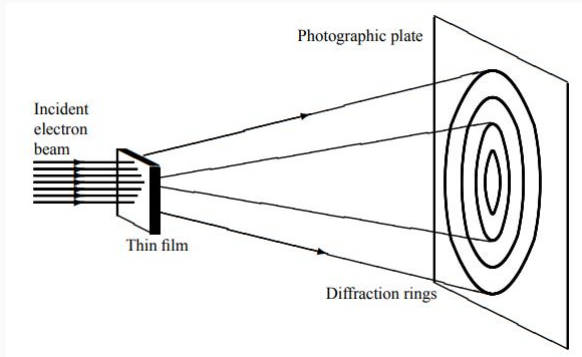
$$h\nu = E_{e^-} + E_{e^+} + E_N$$

$$= (m_e c^2 + k_{e^-}) + (m_e c^2 + k_{e^+}) + K_N$$

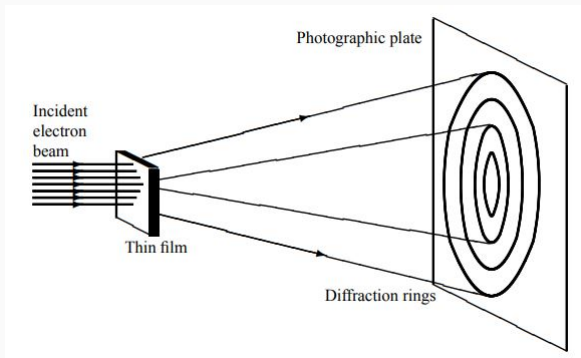
# Wave Aspect of Particles

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# Matter Waves [1923]



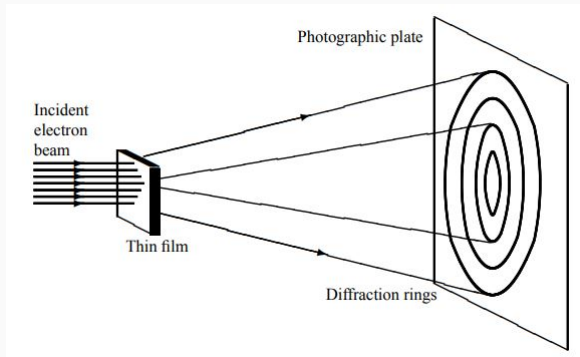
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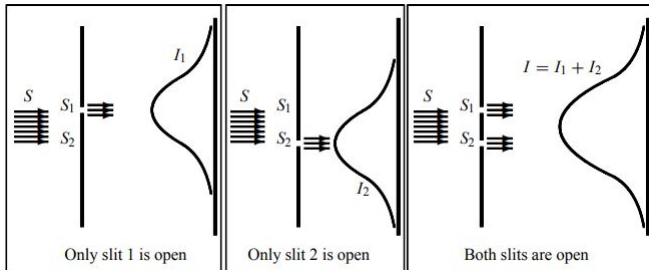
e.g. BuckminsterFullerene (C60) is the largest object observed to exhibit wave-particle duality

# Particles vs Waves

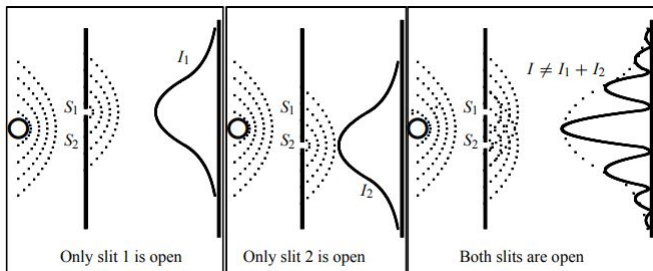
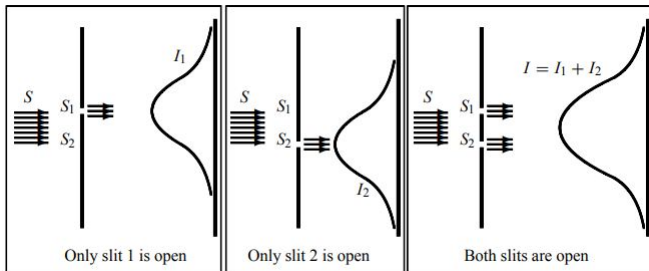
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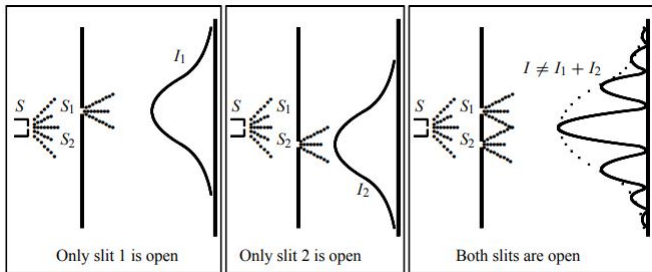
# Classical View of Particles and Waves



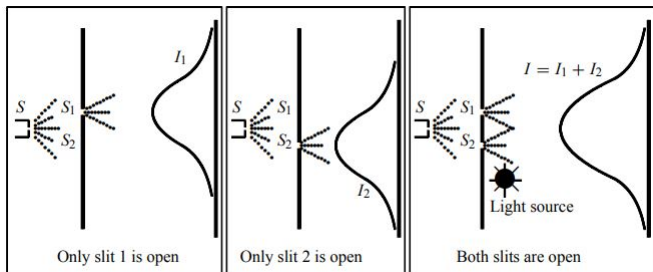
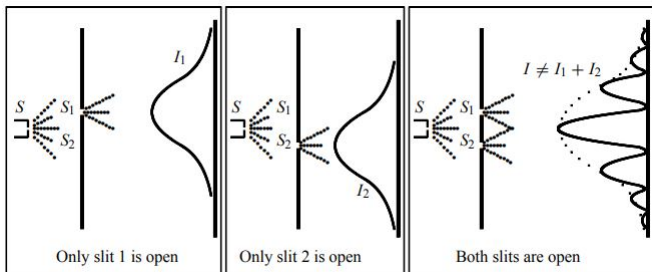
# Classical View of Particles and Waves



# Quantum View of Particles and Waves



# Quantum View of Particles and Waves



# Indeterministic Nature of the Microphysical World

Double-slit experiment shows:

- microscopic material particles do give rise to interference patterns.
- it is impossible to trace the motion of individual electrons.
- electrons display both particle and wave properties.

# Wave–Particle Duality: Complementarity

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- An experiment designed to isolate the particle features of a quantum system gives no information about its wave features, and vice versa
- Particle and wave manifestations do not contradict or preclude one another, they are just **complementary**. Bohr.

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- If a particle is accurately localized (i.e.,  $\Delta x \rightarrow 0$ ), there will be total uncertainty about its momentum (i.e.,  $\Delta p_x \rightarrow \infty$ )

# Probabilistic Interpretation

In quantum mechanics the state (or one of the states) of a particle is described by a wave function  $\psi(\vec{r}, t)$ , corresponding to de Broglie wave of this particle. It describes the wave properties of a particle.

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Max Born interpreted as the probability of finding the particle somewhere in space:

$$\int_{allSpace} |\psi(\vec{r}, t)|^2 d^3r = 1$$

where  $\psi$  is a solution of the Schrödinger equation.

# Classic: Rutherford Atom [1911]



Fails to explain:

- atoms are stable (should lose energy)
- radiate energy over discrete frequency ranges (should emit over continuous range)



# Quantum: Bohr Atom [1913]

Shown by experiment:

- atoms are stable
- radiate energy over discrete frequency ranges
- Only a **discrete** set of circular stable orbits are allowed.
- Emission or absorption of radiation can take place only when an electron jumps from one allowed orbit to another.

# Postulates of Quantum Mechanics

- Spatial distribution of a particle is defined by a wave function.
- A state vector (wave function)  $\psi(\vec{r}, t)$  contains all the information we need to know about the system and from which all needed physical quantities can be computed.
- Quantum postulates cannot be derived; they result from experiment.

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The square norm of wave function  $|\psi(\vec{r}, t)|^2$  represents a position probability density, that is the probability of finding the particle at time  $t$  in a volume element.

# Superposition Principle

- Digression on vectors in  $R^2$
- Superposition of wave functions solutions of Schrödinger equation:

$$\psi(\vec{r}, t) = \alpha_1 \psi_1(\vec{r}, t) + \alpha_2 \psi_2(\vec{r}, t)$$

# Measurement in Quantum Mechanics

- In QM the measurement process perturbs the system significantly.
- The act of measurement generally changes the state of the system



# Computational Quantum Mechanics

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The minimum unit of quantum information is a quantum bit, **qubit**. Is a linear superposition of two orthogonal quantum states:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$$

where  $\alpha$  and  $\beta$  are arbitrary complex values satisfying  $|\alpha|^2 + |\beta|^2 = 1$ .