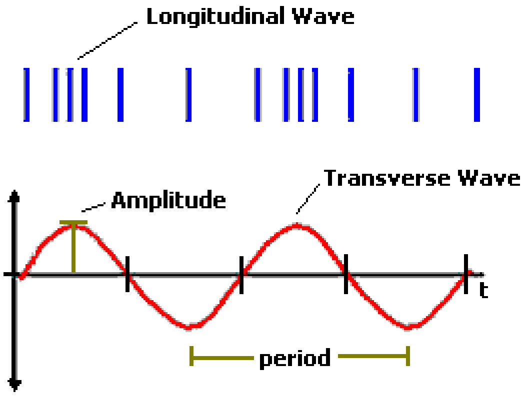
# Introduction to Quantum Mechanics

Quantum mechanics is the theoretical framework which describes the behavior of matter on the atomic scale. It is the most successful quantitative theory in the history of science, having withstood thousands of experimental tests without a single verifiable exception. We review briefly some of the concepts of classical physics as well as failures of classical physics, which brought about the birth of quantum mechanics.

## 1. Classical Waves

### 1.1 Harmonic wave (sinusoidal)



$$\psi(x)=A\cdot\sin(\frac{2\pi x}{\lambda}) \qquad (1)$$

$A$ Amplitude; $\lambda$ wave length

### 1.2 Traveling Waves (animation)

$$\Psi(x,t)=A\cdot\sin[\frac{2\pi(x-ct)}{\lambda}] \qquad (2)$$

Velocity $c$

$$c=\frac{number\ of\ periods}{second}\times\frac{length}{period}=\frac{length}{second}=\nu\lambda \qquad (3)$$

General form:

$$\Psi(x,t)=A\cdot\sin[\frac{2\pi(x-ct)}{\lambda}-\epsilon] \qquad (4)$$

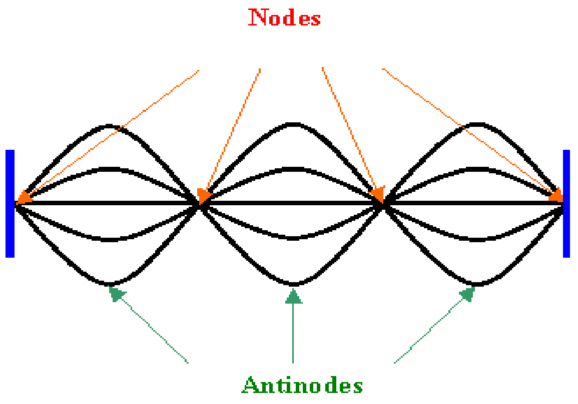
$\epsilon$ Phase factor: $\pi, 3\pi, \ldots(2n+1)\pi$ - out of phase
$2\pi, 4\pi, ..2n\pi$ - in phase

## 1.3 Standing waves (animation)

$$\begin{aligned} \Psi(x,t) &= \Psi_{primary}(x,t)+\Psi_{reflected}(x,t) \\ &= A\cdot\sin[\frac{2\pi(x-ct)}{\lambda}]+A\cdot\sin[\frac{2\pi(x+ct)}{\lambda}] \\ &= 2\mathrm{A}\cdot\sin(2\pi x/\lambda)\cos(2\pi ct/\lambda) \end{aligned} \tag{5}$$

Trigonometric identity:

$$\boxed{\sin(\theta\pm\phi)=\sin(\theta)\cos(\phi)\pm\cos(\theta)\sin(\phi)} \tag{6}$$



Nodes $2\mathrm{A}\cdot\sin(2\pi x/\lambda)=0$ , i.e., $x=n\lambda/2$

Antinodes $x=(n+1/2)\lambda/2$

$$\Psi(x,t)=\psi(x)\cos(\omega t) \tag{7}$$

Profile function $\psi(x)$ , frequency factor $\omega=2\pi c/\lambda$

## 1.4 The classical wave equation

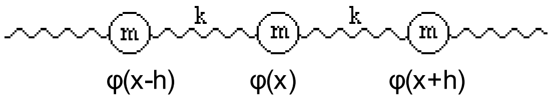
The wave function is a second order linear partial differential equation to describe the propagation of waves: sound waves, fluid waves, light waves. It arises in fields such as acoustics, electro-magnetics, fluids, etc.

$$\frac{\partial^2\Psi}{\partial t^2}=c^2\nabla^2\Psi \tag{8}$$

$\nabla^2$ the Laplacian, $\nabla^2\Psi(x,y,z,t)=\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi(x,y,z,t)$

$c$ wave propagation velocity

**Derivation of the wave equation (1D)**



$\phi(x)$ denotes the distance from the equilibrium of the mass at $x$

$k$ denotes the stiffness of the string

The force exerted on the mass $m$ at $x$ can be expressed as:

$$F_{Newton} = m\vec{a} = m\frac{\partial^2 \psi(x,t)}{\partial t^2} \tag{9}$$

$$F_{Hooke} = F_{x+h} + F_{x-h} = k(\psi(x+h,t) - \psi(x,t)) + k(\psi(x-h,t) - \psi(x,t))$$
$$F_{hooke} = k(\psi(x+h,t) - 2\psi(x,t) + \psi(x-h,t)) = k\frac{\partial^2 \psi(x,t)}{\partial x^2} \tag{10}$$

From Equation (9) and (10)

$$\frac{\partial^2 \psi(x,t)}{\partial t^2} = \frac{k}{m}\frac{\partial^2 \psi(x,t)}{\partial x^2} \tag{11}$$

This is a time-dependent wave equation.

For standing waves, from equation (7) we have

$$d^2\psi(x)/dx^2 = -(\omega^2 m/k)\psi(x) \tag{12}$$

One solution to this differential equation:

$$\psi = A\cdot\sin(\omega\sqrt{(m/k)}\,x) \tag{13}$$

This wave functions gives a wave length of $\omega\sqrt{m/k}\,\lambda = 2\pi$ or,

$$\omega\sqrt{m/k} = 2\pi/\lambda \tag{14}$$

Equation (12) becomes a time-independent wave equation:

$$d^2\psi(x)/dx^2 = -(2\pi/\lambda)^2\psi(x) \tag{15}$$

Likewise, in 3D, the time-independent wave equation is:

$$\nabla^2\psi(x,y,z) = -(2\pi/\lambda)^2\psi(x,y,z) \tag{16}$$

Try to find a solution to this equation for a clamped string.

## 2. Brief History of Quantum Mechanics

- Newtonian Mechanics: Newton's laws of motion and gravitation (1687) *Principia*
- James Clark Maxwell's unification of the phenomena of electricity, magnetism and optics (1864) (perhaps the greatest achievement of physics in the 19th century)
- Heinrich Hertz first produced and detected electromagnetic waves (1887)
- Max Planck proposed energy quanta to explain blackbody radiation (1900)
- Einstein's explanation of photoelectric effect (1905). $E = h\nu$

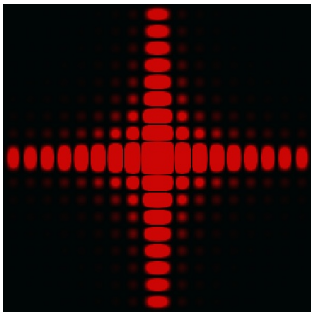
- Neils Bohr's atomic model to explain line spectra. (1913)
- Louis de Broglie's wave-particle duality and matter wave (1922) $\lambda = h/p$
- Werner Heisenberg formulated the uncertainty principle (1925) $\Delta x \cdot \Delta p \geq \hbar/2$
- Max Born and Pascual Jordan invented *matrix mechanics* (1925)
- Erwin Schrödinger introduced *wave mechanics* (1926) $ih\dot{\Psi} = H\Psi$
- Wolfgang Pauli presented a formal theory about the electron spin (1927)
- Paul Dirac reconciled quantum mechanics with the special theory of relativity (1928)
- Richard Feynman devised the path integral formulation of quantum mechanics (1948)

## Light – Waves or Particles?

### 2.1 Corpuscular theory of light

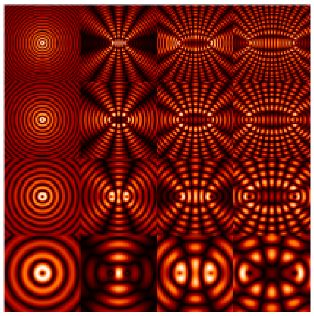
Corpuscular theory of light due to Sir Issac Newton: Light is made up of small discreet particles (called "corpuscles"). It failed to describe *diffraction* and *interference* of light.

Diffraction (bending of lights passing by an obstacle)



Intensity pattern of a light passing through a square

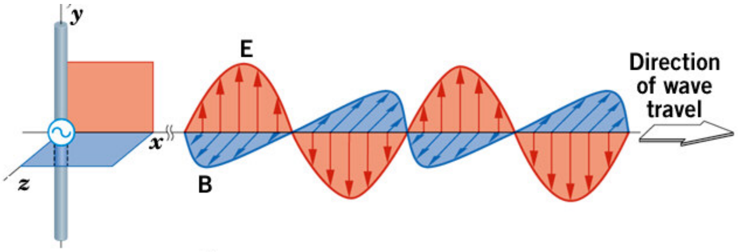
Interference (interaction of diffracted lights)



Interference of circular light waves

### 2.2 Electromagnetic waves

Maxwell's electromagnetic wave theory:



Electromagnetic waves consist of mutually perpendicular electric and magnetic fields, $\boldsymbol{E}$ and $\boldsymbol{B}$ respectively, oscillating in synchrony and propagating in the direction of $\boldsymbol{E} \times \boldsymbol{B}$ (right-hand rule), at the *speed of light* $c = 2.9979 \times 10^8$ m/second:

$$\lambda \nu = c \tag{17}$$

Electromagnetic radiation exists in a wide range of wavelength: radio waves, microwaves, infrared radiation, visible light, ultraviolet radiation, X-rays, Gamma rays.

The energy density of an electromagnetic field in free space (in the absence of dielectric and magnetic media) is given by: $\rho_E = \frac{1}{2}\left(\epsilon_0 E^2 + \mu_0^{-1} B^2\right)$ .

Define the amplitude of an electromagnetic wave at each point in space $\vec{r}$ at time t:

$$\Psi(\vec{r},t) = \sqrt{\epsilon_0}\, E(\vec{r},t) = \frac{B(\vec{r},t)}{\sqrt{\mu_0}}$$

$$\rho(\vec{r},t) = \left|\Psi(\vec{r},t)^2\right| = \Psi^*(\vec{r},t)\,\Psi(\vec{r},t) \qquad (18)$$

$\Psi^*(\vec{r},t)$ Is the complex conjugate of $\Psi(\vec{r},t)$

## 2.3 Three failures of classical physics

- Ultraviolet catastrophe (blackbody radiation)

A red-hot object can emit radiation of a sequence of wavelengths. Classic physics assumes the energy of oscillators does not depend on wavelength. It follows, you would get a sunburn while drinking a cup of coffee (due to the contribution of ultraviolet light).

Planck showed that radiation came only in packets or quanta of a certain size.

$$E = h\nu \qquad (19)$$

$h$ : Planck's constant, $6.626\times 10^{-34}$ Jsec.

The energy in the packets or quanta, is higher for ultraviolet and x-rays, than for infrared or visible light. This means that unless a body is very hot, like the Sun, it will not have enough energy, to give off even a single quantum of ultra violet or x-rays.

- Photoelectric effect

Visible or ultraviolet light impinging on clean metal surfaces can cause electrons to be ejected from the metal. The velocity of the electrons (energy) does not depend on the intensity of the light, which can not be explained by the electromagnetic theory.

Einstein's explanation: Light consists of *photons* with each of energy $h\nu$ .

Q: What is the momentum ( $p$ ) of a photon with a wavelength of $\lambda$ ?

A: According to the equation of atomic energy (theory of relativity) $E = mc^2$ , i.e., $m = \frac{E}{c^2}$ . Thus, the momentum of a photon $p = mv = \frac{E}{c^2}v = \frac{h\nu v}{c^2}$ . if we let $v = c$ , we obtain:

$$p = \frac{h\nu}{c} = \frac{h}{\lambda} \qquad (20)$$

- Line spectra

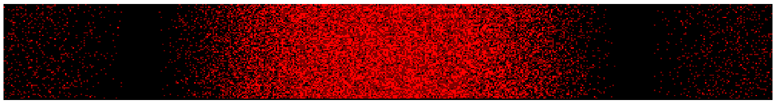
According to classical electrodynamics, an accelerated electric charge will emit radiation. If we accept Rutherford's model of hydrogen atom, we would expect a continuous emission of radiation and hence a continuous loss of energy by the electrons. This would result in the orbit getting smaller and smaller.

Fact: Discreet line spectra lines.

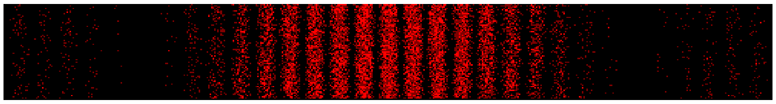
Bohr's model: $E_1 - E_2 = h\nu$
Bohr frequency rule: ground state and excited states. (successful for the line spectrum of hydrogen)

### 2.4 Wave-particle duality

Single-slit



Double-slit



Under appropriate circumstances light can behave either as a wave or as a particle.

De Broglie first conjectured that matter might also exhibit a wave-particle duality, such as electrons. A general equation relating particle momentum $p$ and associated wavelength $\lambda$ (The first person received a Nobel prize based on a Ph.D thesis):

$$p = h/\lambda \tag{21}$$

This theoretical suggestion received experimental confirmation in 1927, when Davisson and Germer at Bell Labs observed the diffraction of a beam of electrons by a crystal of nickel.

Q: What is the de Broglie wavelength of an electron that has been accelerated from rest through a potential change of 500 V?

### 2.5 The Heisenberg uncertainty principle

$$\Delta x \cdot \Delta p \geq \hbar/2$$

“Does God play dice with the universe?” -- Einstein's quote
Einstein-Podolsky-Rosen paradox (Quantum entanglement)

## 3. Schrödinger's Time-independent Wave Equation

### 3.1 Transition from classical mechanics to quantum mechanics

Clever modifications to a classical expression, to get its quantum-mechanical equivalent.

**Example 1:**

The classical Hamiltonian function of a conservative system consists of momentum $p$

and positional coordinate $x$, denoted by $H(x,p)$

The classical energy equation in Hamiltonian form is:

$$H(p,x)=E \tag{22}$$

Where, $E=\frac{1}{2}mv^2+V(x)=p^2/2\mathrm{m}+V(x)$

The de Broglie wavelength $\lambda=\frac{h}{\sqrt{2\mathrm{m}(E-V)}}$

According to the classical wave equation:

$\nabla^2\psi=-(\frac{2\pi}{\lambda})^2\psi$, we have $(\frac{\lambda}{2\pi})^2\nabla^2\psi=-\psi$. Therefore,

$$[\frac{-\hbar^2}{2\mathrm{m}}\nabla^2+V]\psi=E\cdot\psi \tag{23}$$

$$\frac{p^2}{2\mathrm{m}}+V=E \tag{24}$$

Two operators:

Hamiltonian operator: $\hat{H}\psi=E\psi$ , $\hat{H}\Leftrightarrow-\frac{\hbar^2}{2\mathrm{m}}+V$

momentum operator: $\hat{p}_x\Leftrightarrow\frac{\hbar}{i}\frac{\partial}{\partial x}$

**Example 2:**

Euler's formula: $e^{\pm i\theta}=\cos\theta+i\sin\theta$

Consider a wave function of the form: $\Psi(x,t)=\exp[2\pi i(\frac{x}{\lambda}-\nu t)]$

Replace $\nu$ and $\lambda$ by their particle analogs (Planck and de Broglie formula):

$\nu=\frac{E}{h}$ , $\lambda=\frac{h}{p}$ :

$$\Psi(x,t)=\exp[i(px-Et)/\hbar] \tag{25}$$

Reverse engineering: From wavefuntion $\Rightarrow$ wave equation $\frac{\partial\Psi}{\partial t}=?$

$$i\hbar\frac{\partial\Psi}{\partial t}=E\Psi=H\Psi \tag{26}$$

Time-dependent Schrödinger Equation:

$$\Psi(\vec{r},t)=\psi(\vec{r})e^{-iEt/\hbar} \tag{27}$$

## 3.2 Eigenequations

$$\hat{H}\psi = E\psi \quad \Rightarrow \quad Operator\,\psi = const\,\psi$$

Eigenvalue equation: The Schrödinger equation is the best known eigenvalue equation. "Eigenvalue" : a word hybrid with German, meaning "characteristic value".

**E**igenfunctions, or eigenstates, or wavefunctions, or state function $\psi$

### 3.3 Conditions on wavefunction $\psi$

The wavefunciton $\psi(\vec{r})$ : Amplitude of the still vaguely defined matter wave. The most accepted interpretation of the wavefunction is due to Max Born (1926): $\rho(\vec{r})$ , the square of the absolute value of $\psi(\vec{r})$ is proportional to the probability density (probability per unit volume) that the particle will be found at the position $\vec{r}$ . ***Copenhagen Interpretation***

- For a single particle wave, normalized wavefunction: $\int |\psi(\vec{r})^2| d\tau = 1$
- Square-integrable: single-valued, nowhere infinite, piecewise continuous first derivatives.
- Kinetic energy and wiggliness

## PROBLEMS:

1. The equation for a standing wave in a string has the form $\Psi(x,t) = \psi(x)\cos(\omega t)$
(i) Calculate the time-average potential energy (PE) for this motion. [*Hint:* Use PE = $-\int F\,d\Psi \;\; ; \;\; F = ma \;\; ; \;\; a = \partial^2\Psi/\partial t^2$ ]
(ii) Calculate the time-averaged kinetic energy (KE) for this motion. [*Hint:* Use KE = $\frac{1}{2}mv^2$ and $v = \partial\Psi/\partial t$ ]
(iii) Show that this harmonically vibrating string stores its energy on the average half as kinetic and half as potential energy, and that $E(x)_{av} \propto \psi^2(x)$ .

2. The diameter of an atomic nucleus is of the order of $10^{-13}$ cm. You want to obtain information about the size and shape of nuclei and you have decided to do this by bombarding them with fast protons. What is the approximate energy to which you have to accelerate the protons?

3. A certain one-dimensional quantum system in $0 \le x \le \infty$ is described by the Hamiltonian $\hat{H} = \frac{-\hbar^2}{2\mathrm{m}}\frac{d^2}{dx^2} - \frac{q^2}{x}$ ( $q = constant$ ), one of the eigenfunctions is known to be $\psi(x) = Axe^{-\alpha x}, \alpha \equiv mq^2/\hbar^2, A = constant$
(i) Write down the Schrödinger equation and carry out the differentiation.
(ii) Find the corresponding energy eigenvalue (in terms of $\hbar$ , $m$ and $q$ ).
(iii) Find the value of A which normalizes the wavefunciton. [*Hint:* $\int_0^\infty x^n e^{-ax}dx = n!/a^{n+1}$ ]