QUANTUM MECHANICS

General Chemistry I, Lecture Series 5

Pengxin Liu

Reading:
OGC8 §4

Outline Quantum mechanism of MATTER

- The wave nature of electrons
  - de Broglie wave
  - The uncertainty principle

- Wave Function
  - Wave mechanics (波动力学)
  - Particle in A Box
  - Interpretation

Electron: Particle or Wave?

if waves (photons) could behave as particles, as demonstrated by the photoelectric effect, then the converse, namely that particles could behave as waves, should be true.

Any particle that moves at or near the speed of light has kinetic energy given by Einstein's special theory of relatively. In general, a particle of mass m and momentum p has an energy

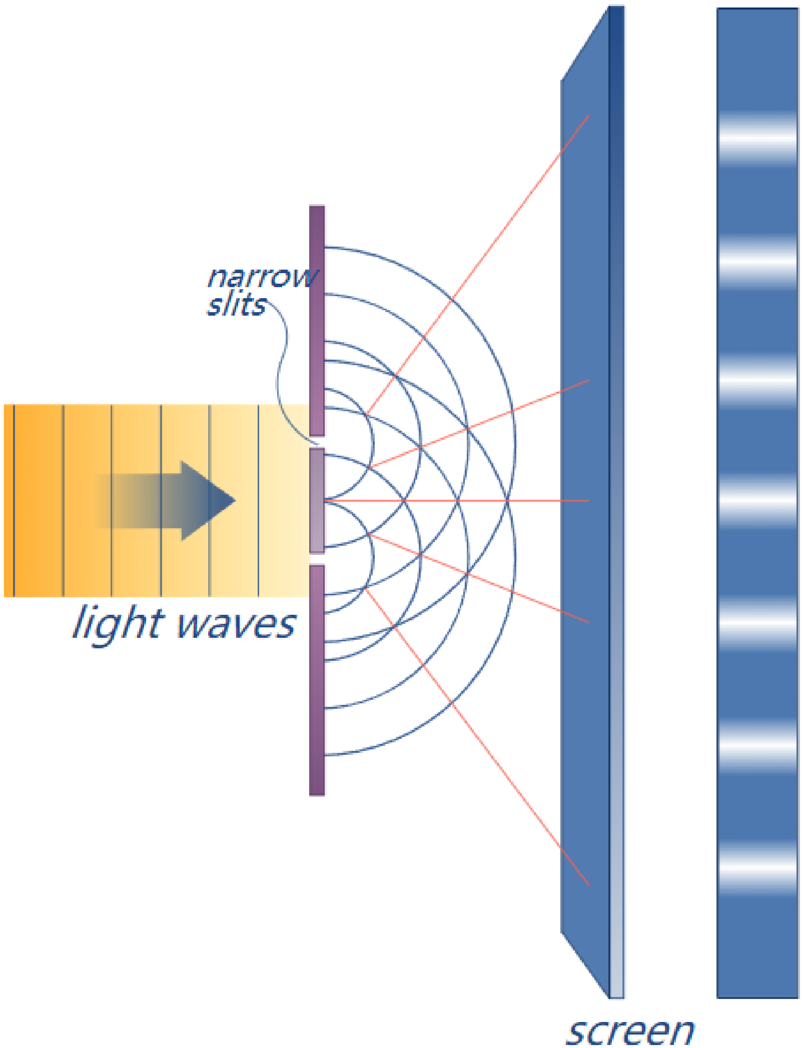
$$E = \sqrt{p^2c^2 + m^2c^4}$$

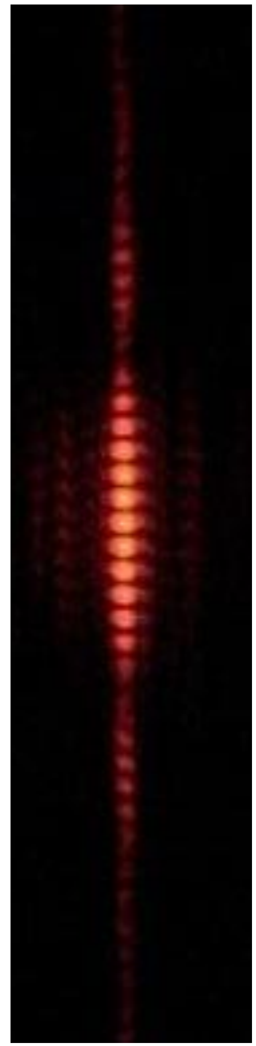
When m=0 **E=** $h\nu = \frac{hc}{\lambda} = pc$

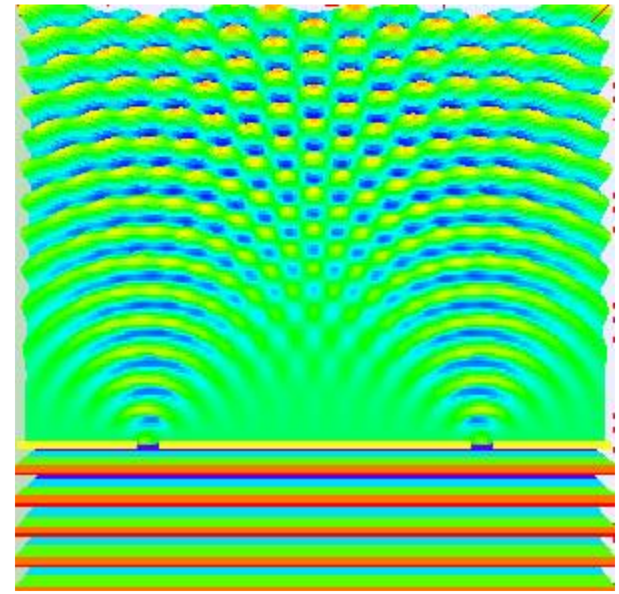
$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

Louis de Broglie (Sorbonne, 1892–1987)

Interference of light







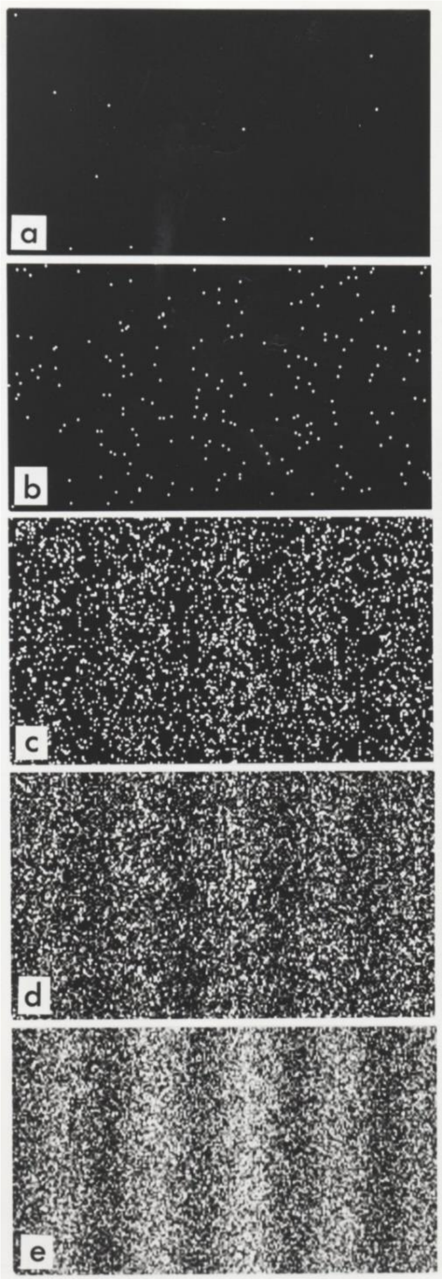
Double-slit interference

Thomas Young in 1801, as a demonstration of the wave behavior of light.

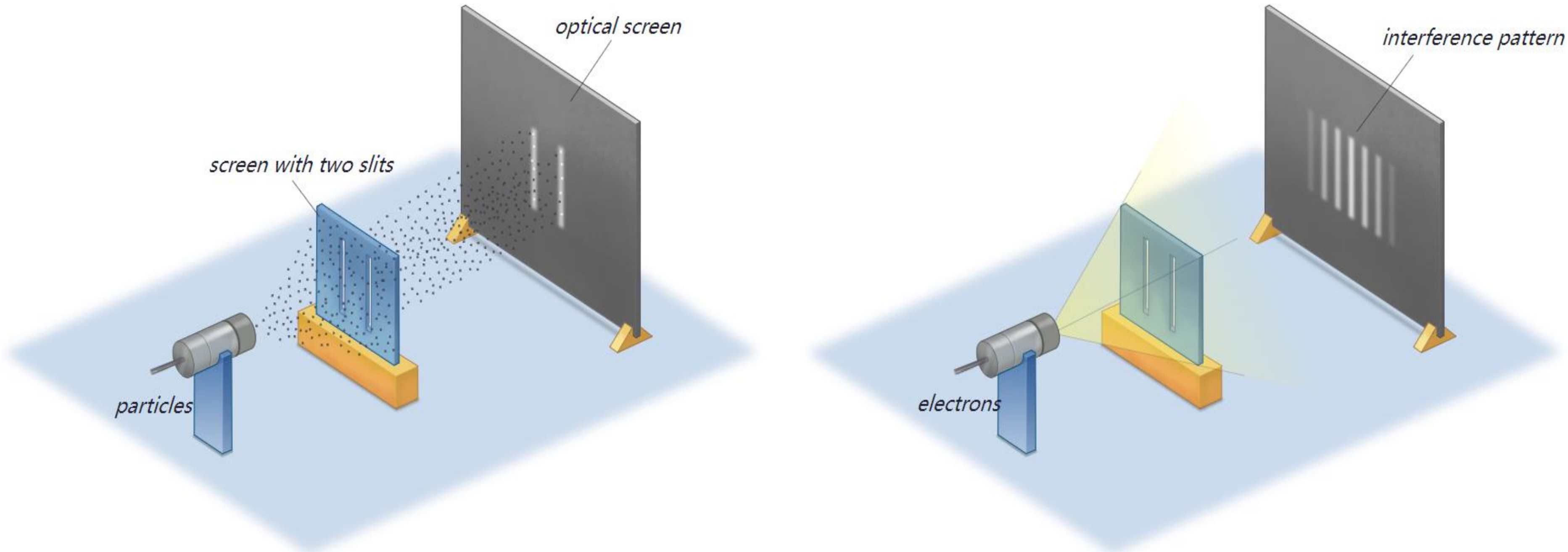
Interference of electrons

G.P. Thomson
(1892-1975)
Son of J. J. Thomson
Interference of electrons 1926

C. Davisson and L. H. Germer in 1927



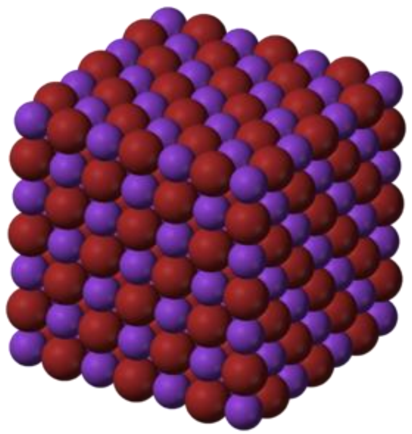
Electron: Particle or Wave?



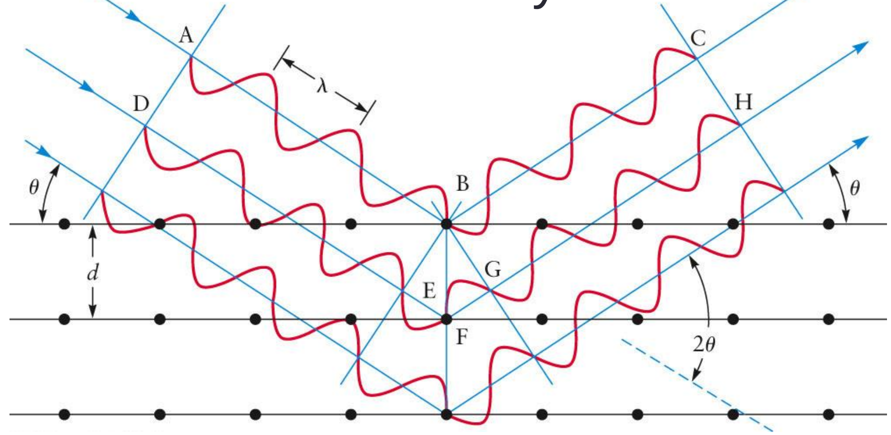
Electrons have **wave-particle duality**, just like photons, in agreement with de Broglie's hypothesis discussed previously.

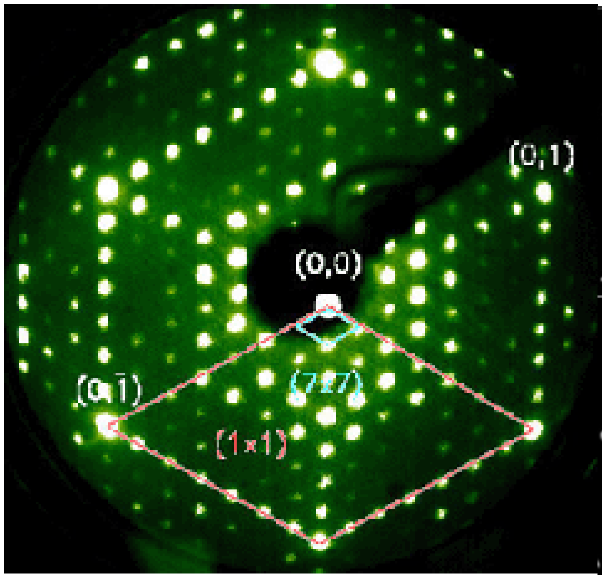
They must have properties like wavelength and frequency.

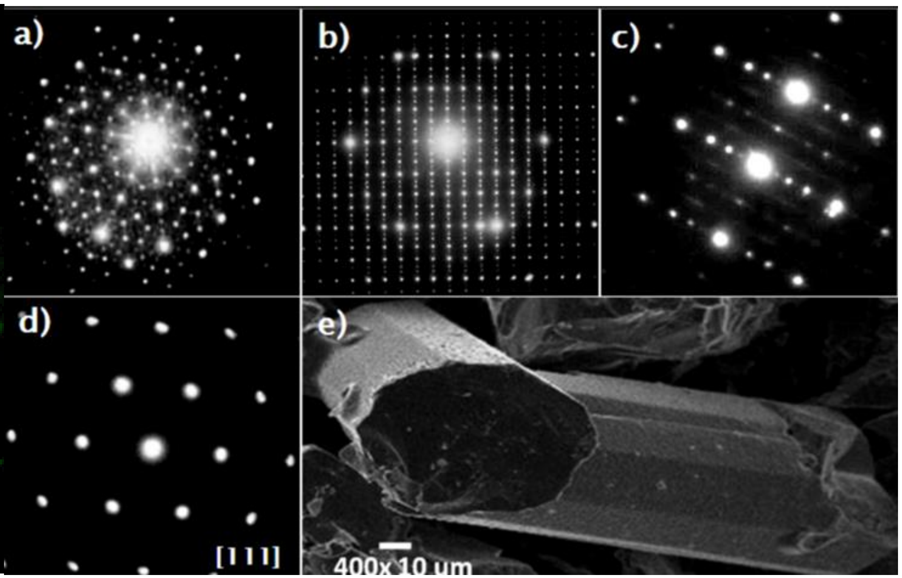
Electron Diffraction Patterns



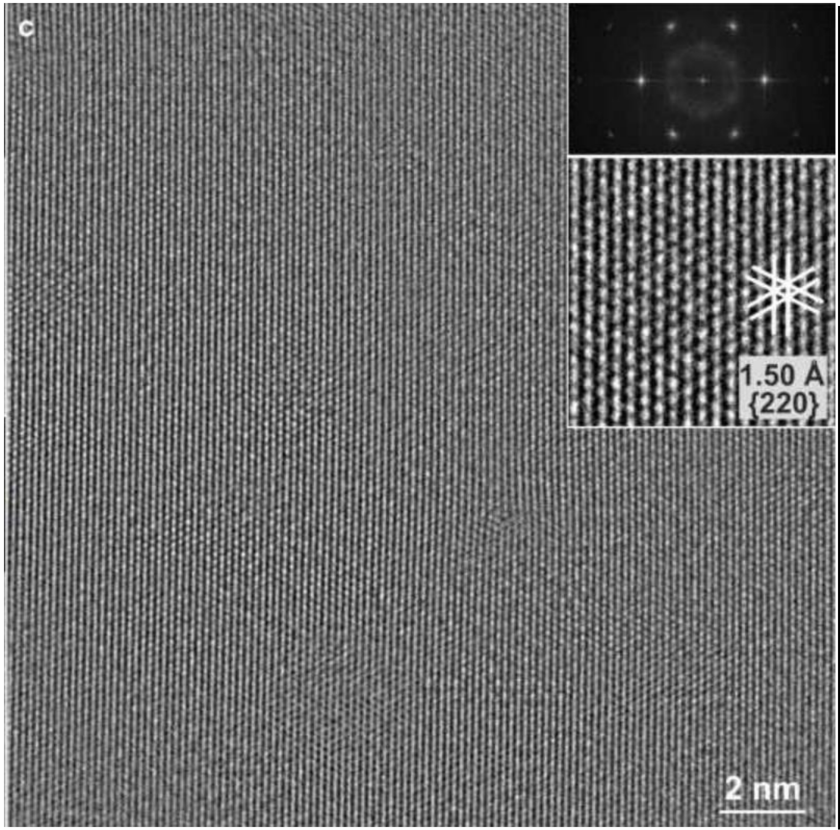
Diffraction of a crystal lattice

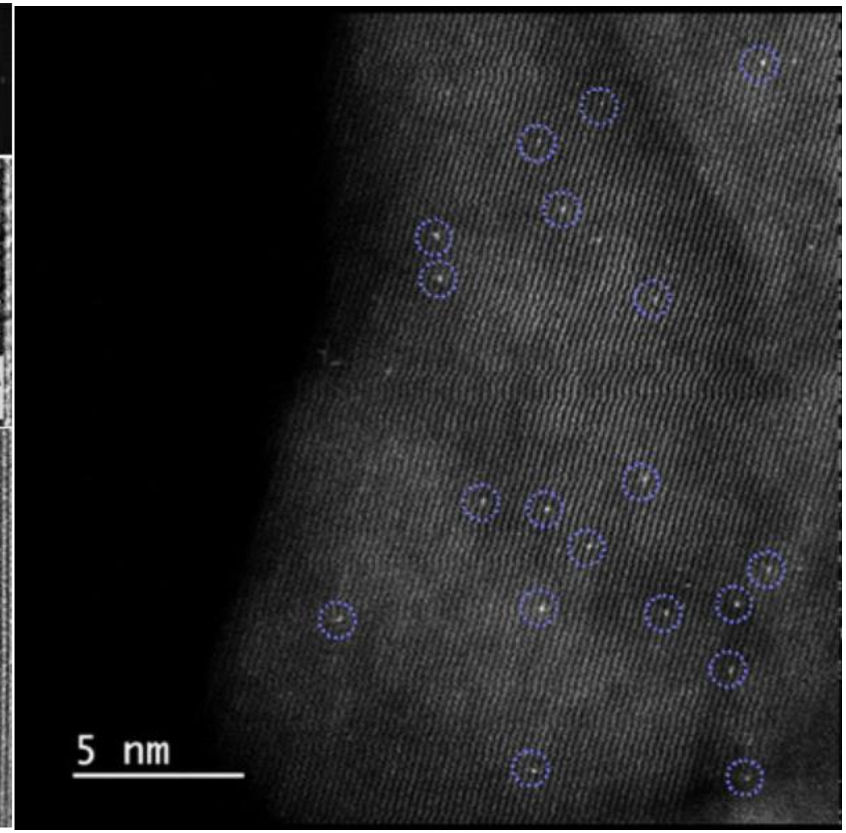






Electron Diffraction Patterns

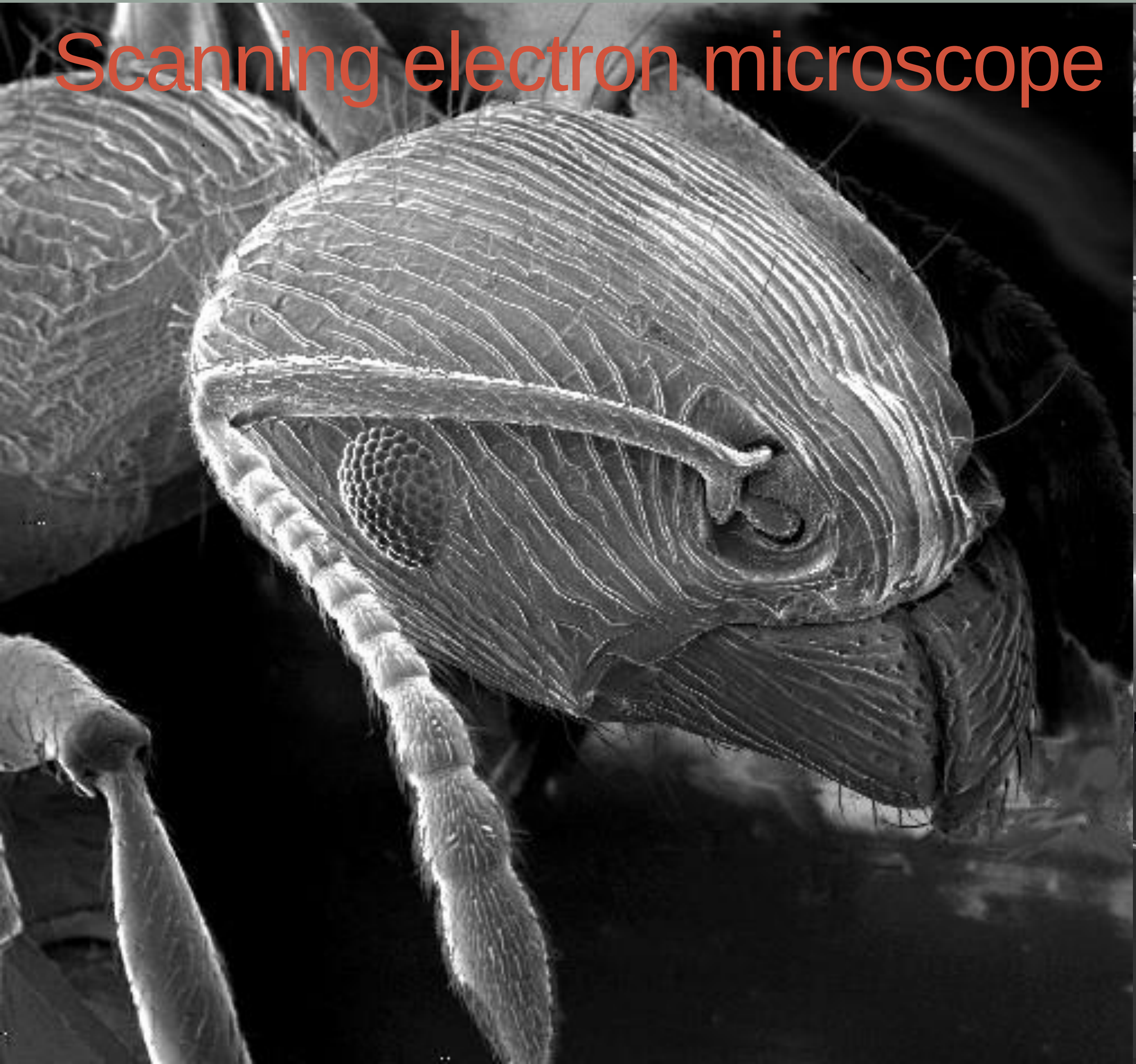


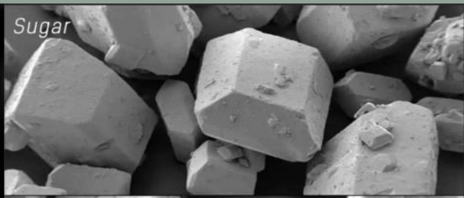


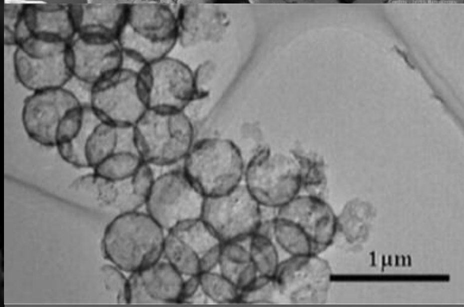
Pengxin Liu*; Paula M. Abdala; Guillaume Goubert; Marc-Georg Willinger*; Christophe Copéret*, ***Angew. Chem. Int. Ed.*** 2021**,** 60, 3254-3260 **(Hot Paper)**

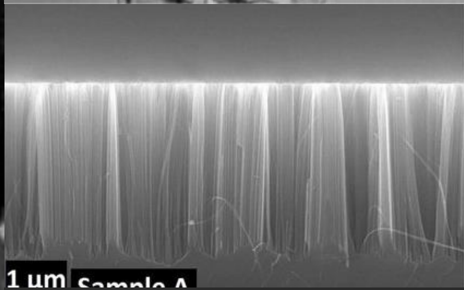
Pengxin Liu*; Xing Huang; Deni Mance; Christophe Copéret*, ***Nature Catalysis***, 2021, 4, 968–975

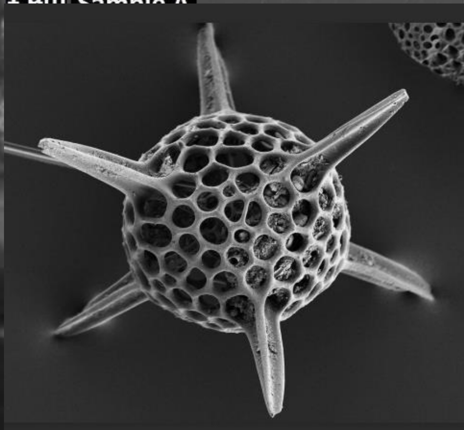
Scanning electron microscope



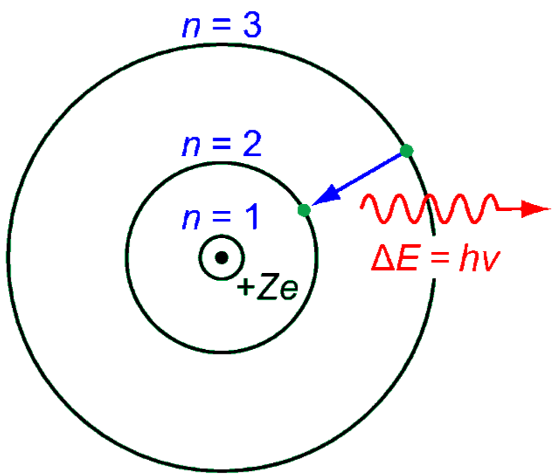




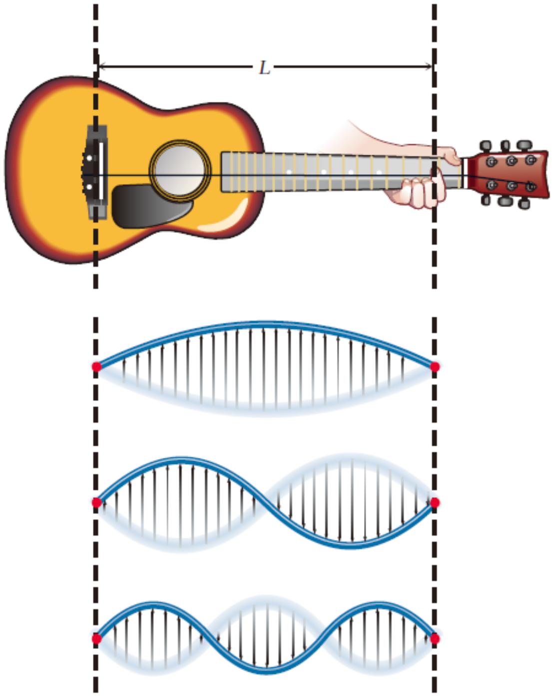




The de Broglie Waves of Electron

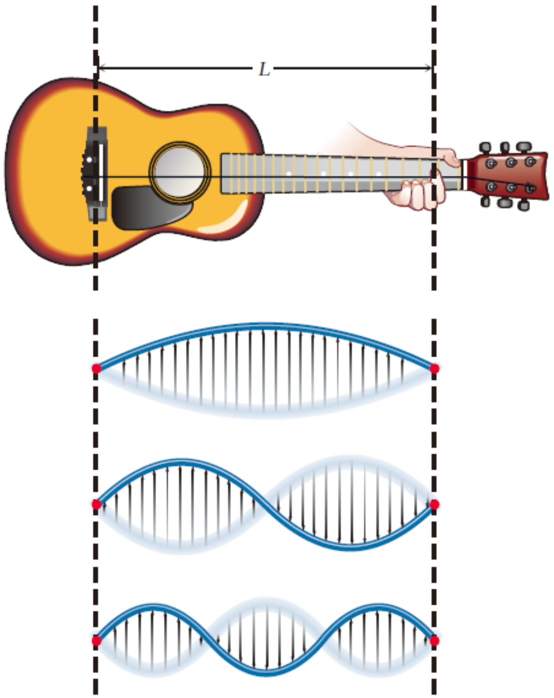


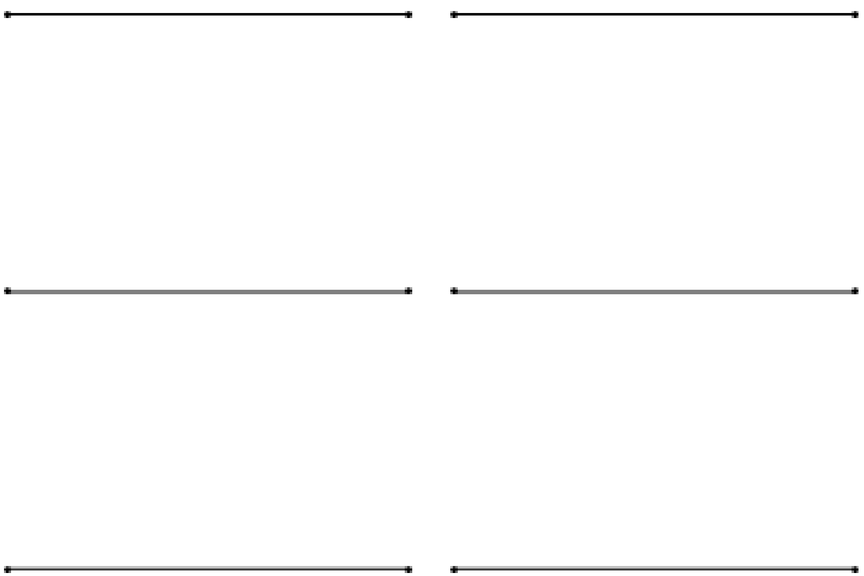
Stationary state
定态



Standing wave
驻波

Standing wave





Linear Standing Waves

Nodes (节点): 0-6

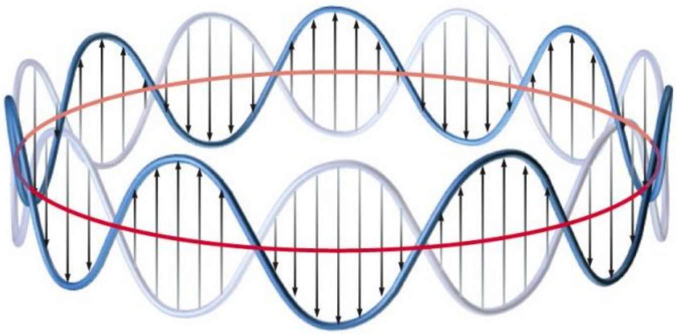
Fixed ends: boundary condition.

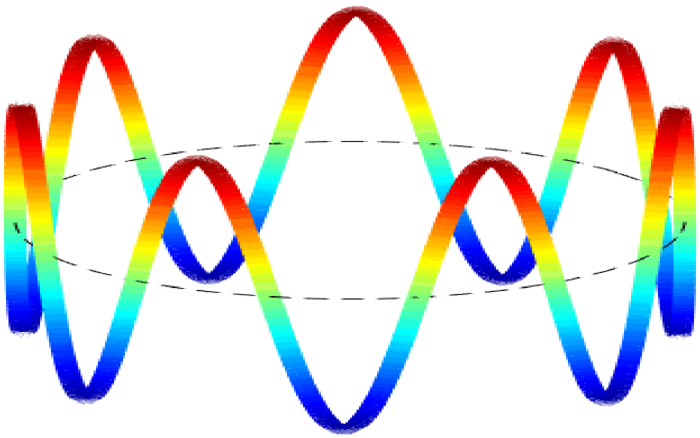
Where oscillation is zero, it's called a node (except for ends)

Standing wave

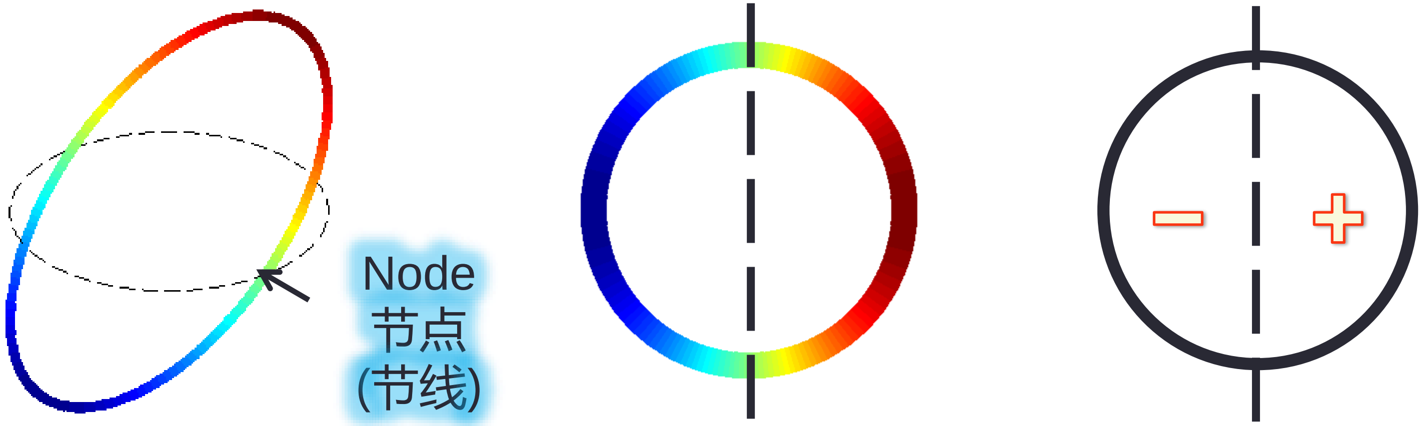
龙洗盆

Circular Standing Waves

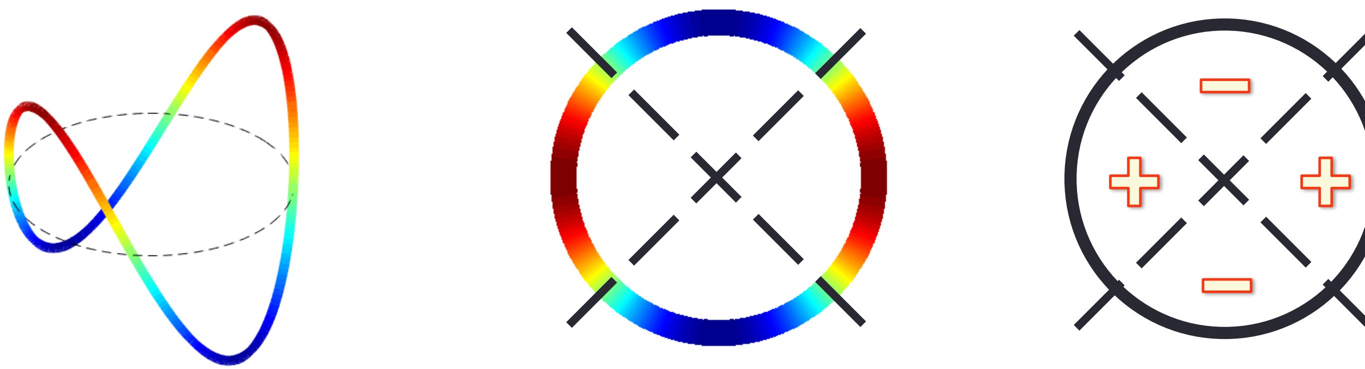




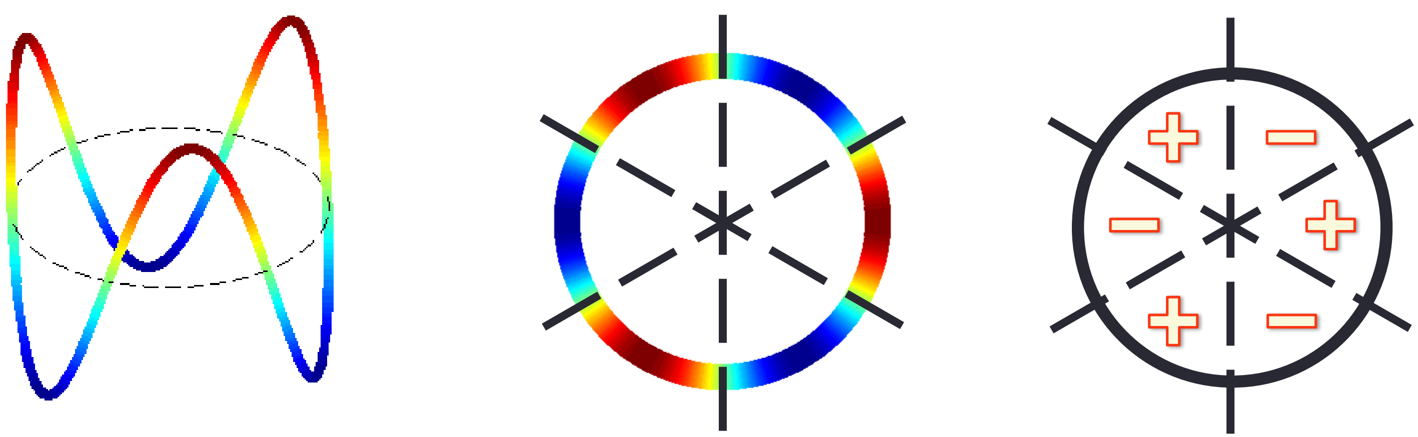
$2\pi r = \lambda$



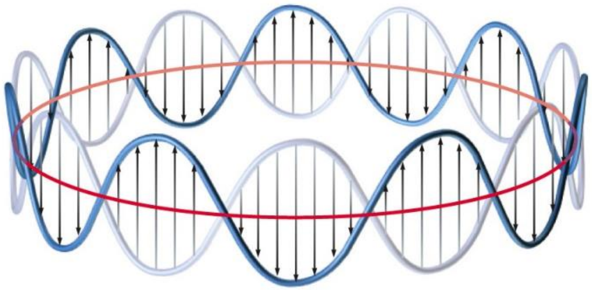
$2\pi r = 2\lambda$



$2\pi r = 3\lambda$



The Wavelength of Electron



$2\pi r = 7\lambda$

(1) Bohr 1913:

$$L = m_e v r = n\frac{h}{2\pi}$$

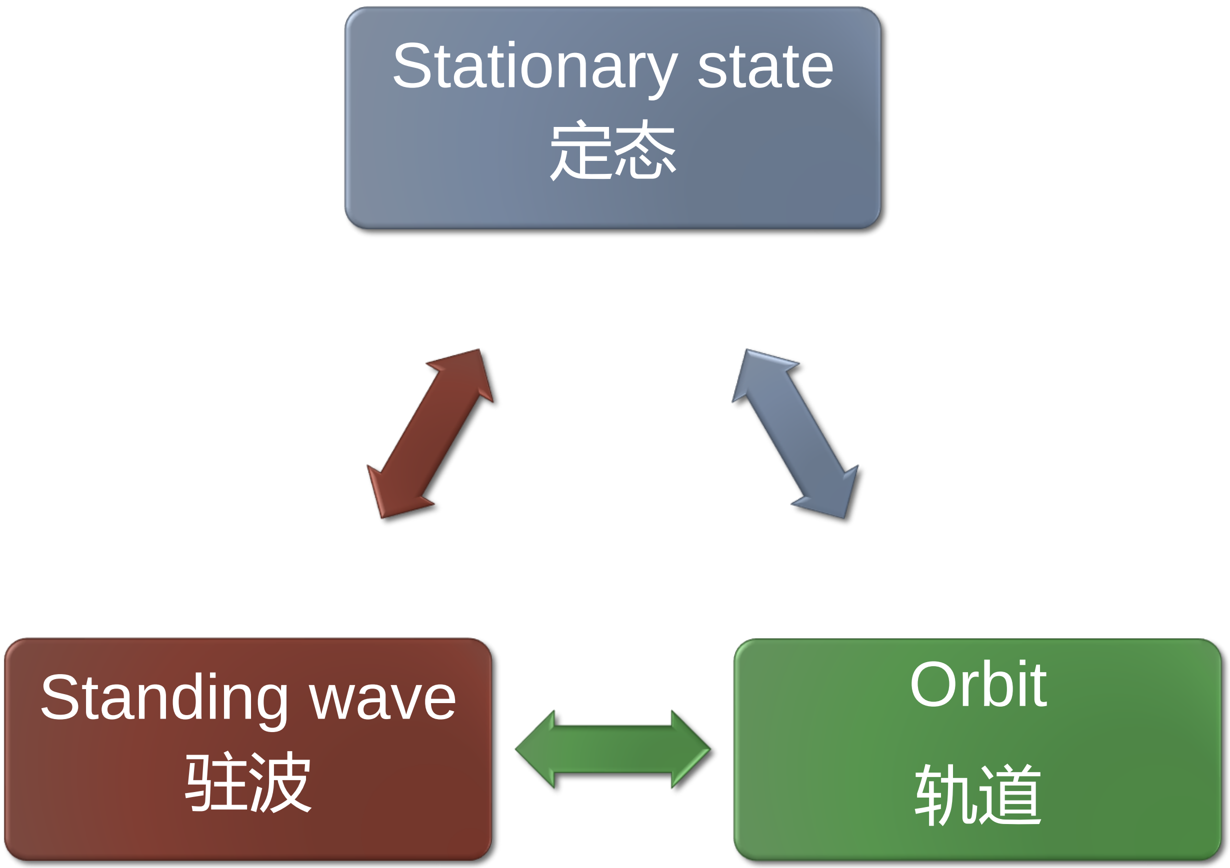
(2) de Broglie 1924:

$$2\pi r = n\lambda$$

(1)+(2)

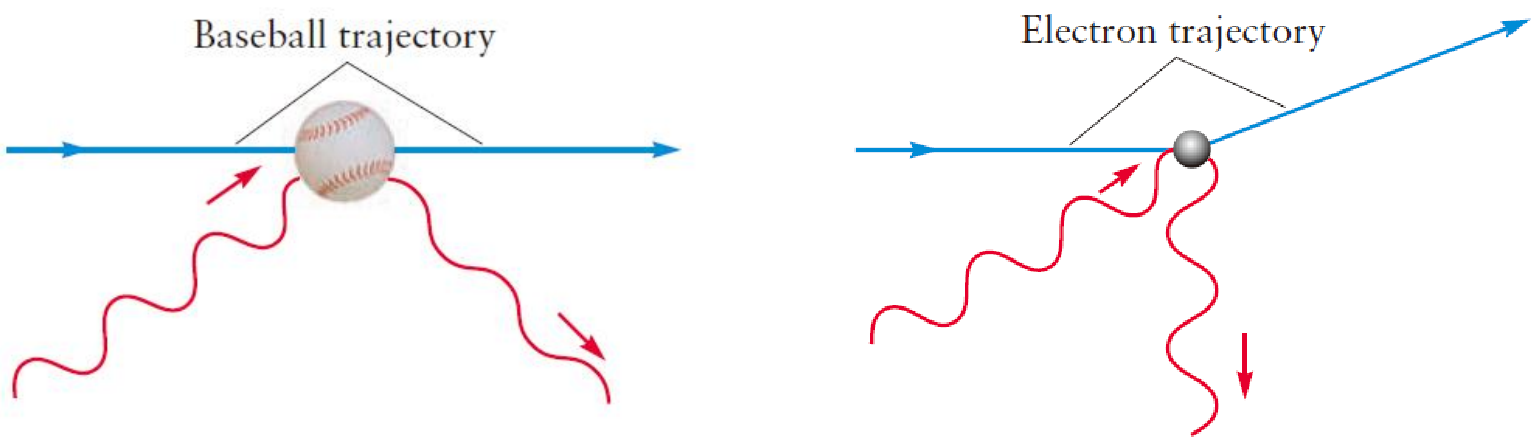
$$p = m_e v = \frac{h}{\lambda}$$

Summary



The Uncertainty Principle

“at every moment the electron has only an inaccurate position and an inaccurate velocity, and between these two inaccuracies there is this uncertainty relation.”



The Uncertainty Principle

Werner Heisenberg (Copenhagen, Leipzig, 1901–1976)

For photon, $p = \frac{hv}{c} = \frac{h}{\lambda}$

For electron, $p = m_e v = \frac{h}{\lambda}$

Common trend:

$$p\lambda = h$$

Heisenberg 1927:

$$\Delta p \cdot \Delta x \geq \frac{h}{4\pi}$$

Standard deviation
标准差

Outline

- The wave nature of electron
  - de Broglie wave
  - The uncertainty principle

- Waves Function
  - Wave mechanics (波动力学)
  - Particle in A Box
  - Interpretation

Quantum mechanics

- Wave mechanics (in comparison to matrix mechanics)
- to describe the energies and spatial distributions of electrons in atoms and molecules.

a mathematical technique that describes the relationship between the motion of a particle that exhibits wavelike properties (such as an electron) and its allowed energies.

Erwin Schrödinger
(Zürich, 1887–1961)
Nobel Prize in Physics, 1933

Schrödinger Equation

- considering a particle moving freely in one dimension with classical momentum, p

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

$$\frac{d\psi(x)}{dx} = A \frac{2\pi}{\lambda} \cos \frac{2\pi x}{\lambda}$$

$$\frac{d^2\psi(x)}{dx^2} = -A\left(\frac{2\pi}{\lambda}\right)^2 \sin \frac{2\pi x}{\lambda} = -\left(\frac{2\pi}{\lambda}\right)^2 \psi(x) = -\left(\frac{2\pi}{h} p\right)^2 \psi(x)$$

$$-\frac{h^2}{8\pi^2 m} \frac{d^2\psi(x)}{dx^2} = \frac{p^2}{2m}\psi(x) = \mathcal{T}\psi(x)$$

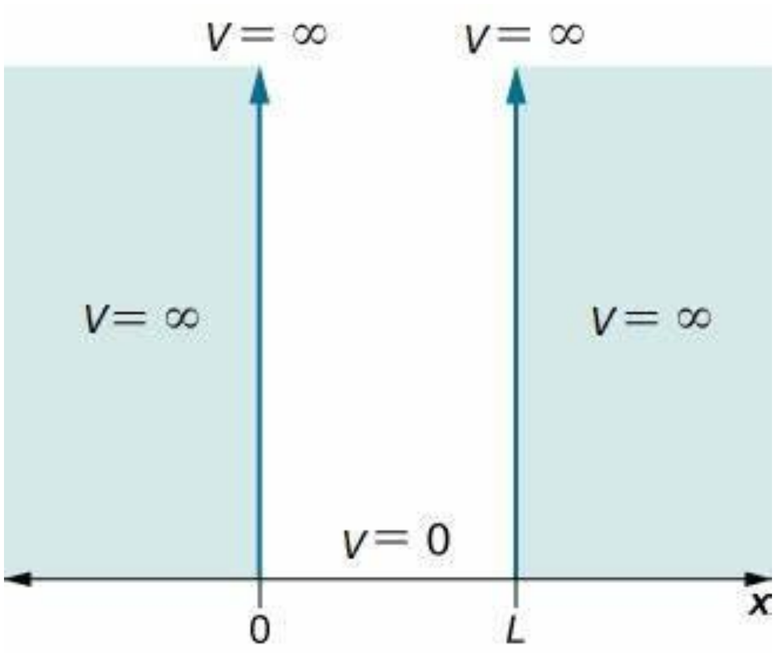
$\mathcal{T} = p^2/2m$ is the kinetic energy of the particle

$$-\frac{h^2}{8\pi^2 m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

Particle in A Box 一维式箱

(1) $\psi(x) = 0$ for $x \leq 0$ or $x \geq L$ (Boundary condition 边界条件)

(2) $\int |\psi(x)|^2 \, dx = 1$

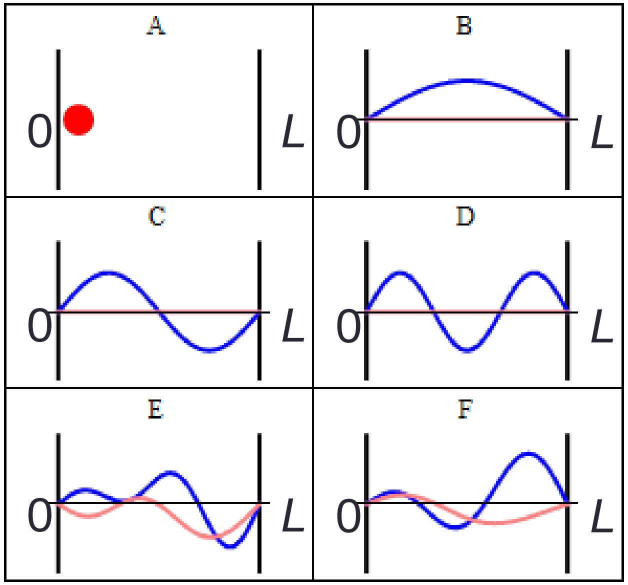


Particle in A Box 一维式箱

$$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

When V = 0 $$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{8\pi^2 mE}{h^2}\psi(x)$$



From Pg 25, sin function might work.
(actually cos also works)

Apply boundary conditions: $\psi(0) = 0$
Now only sin function works

$$\psi(x) = A \sin kx$$

Apply boundary conditions: $\psi(L) = 0$ $\quad kL = n\pi \qquad n = 1, 2, 3, \ldots$

$$\psi(x) = A \sin\left(\frac{n\pi x}{L}\right) \qquad n = 1, 2, 3, \ldots$$

Particle in A Box 一维式箱

wave function must be normalized

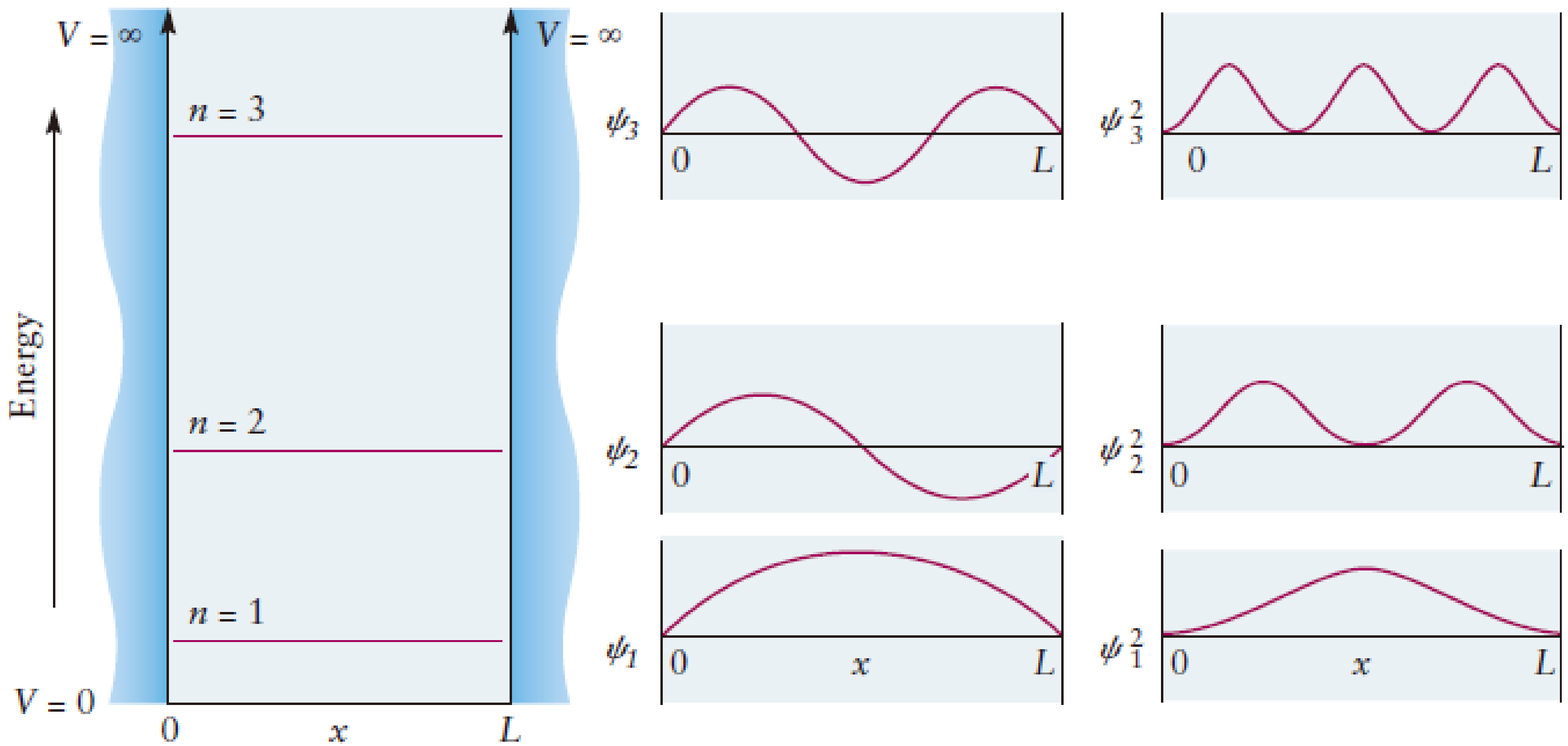
$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$A = \sqrt{\frac{2}{L}}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) n = 1, 2, 3, \ldots$$

$$E_n = \frac{n^2 h^2}{8mL^2} \qquad n = 1, 2, 3, \ldots$$

Particle in A Box 一维式箱



(a) Energy levels (b) Wave functions (c) Probabilities

Interpretation of the Schrödinger Equation

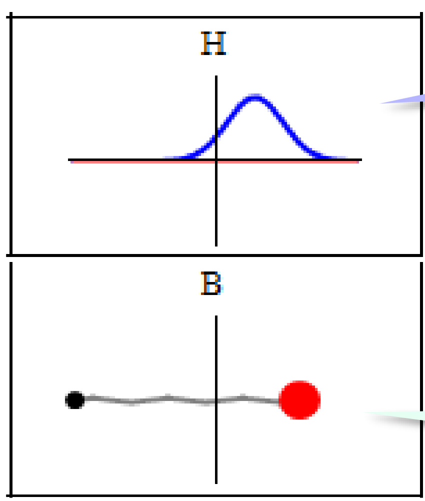
- It is generally considered to be among the most accurate theories of nature because of this astonishingly good agreement.

- Energy quantization is a natural consequence of the Schrödinger equation. States described by these time-independent wave functions are called stationary states.

Wave Function for Electrons

- A function of position *x* and time *t*
- Has a real part and an imaginary part, in general
- Is governed by the Schrödinger Equation (1926)
  薛定谔方程

Real
Imaginary



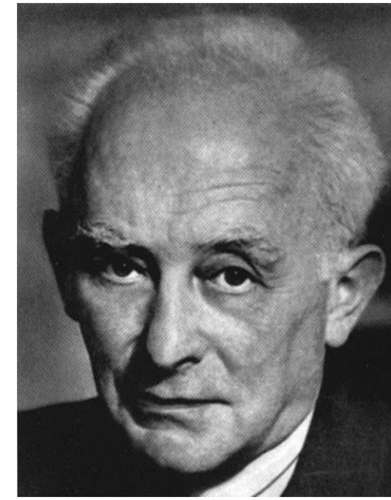
Follows
the Schrödinger Equation

Follows
Newton's Laws

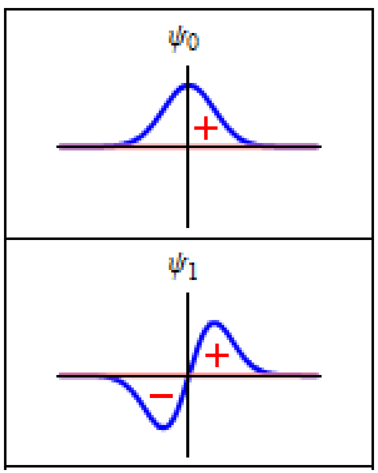
Interpretation of Wave Functions

Probability: $P(x) = |\psi(x)|^2$

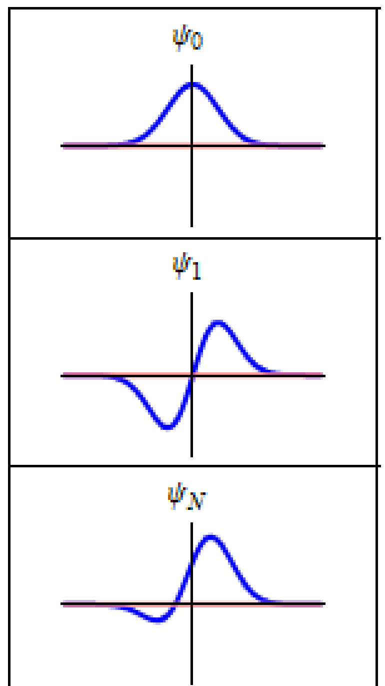
Normalization: $\int |\psi(x)|^2 \, dx = 1$
归一化



Max Born (Göttingen, 1882–1970)



Textbook notation



Stationary states
定态

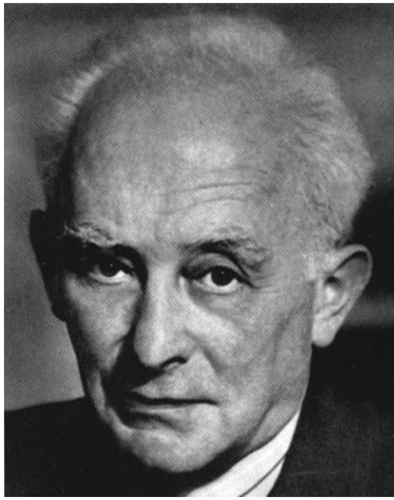
Time-dependent state

Interpretation of Wave Functions

Probability: $P(x) = |\psi(x)|^2$

Normalization: $\int |\psi(x)|^2\, dx = 1$

归一化



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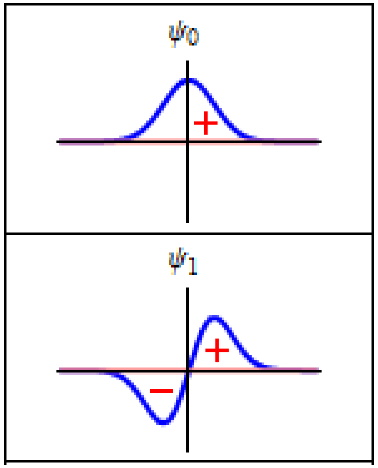
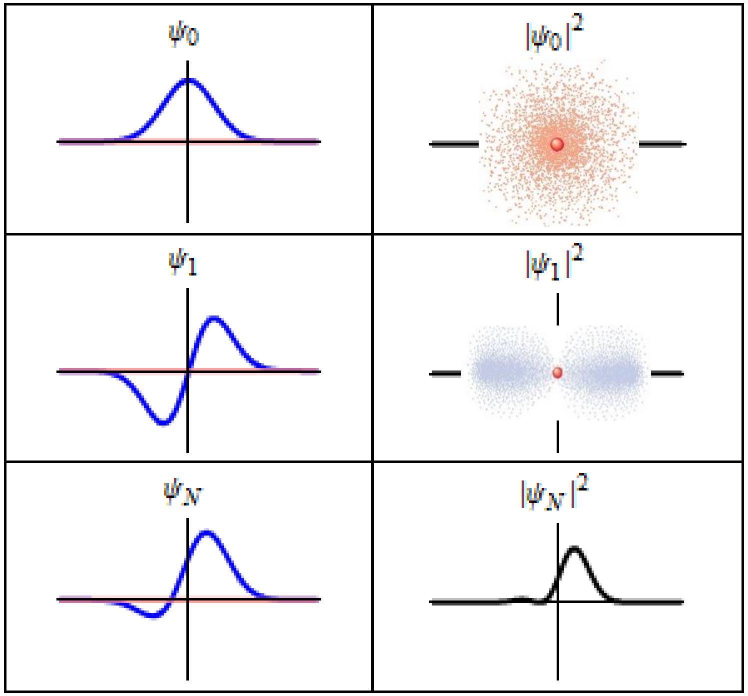


Textbook notation



Stationary states
定态

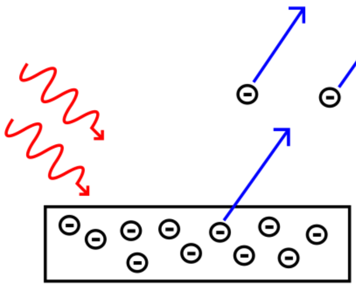
Time-dependent state

Physical meaning of the Schrödinger Equation

- Quantum mechanics do not care about where is a particle, but care about the probability of finding a particle at given space.

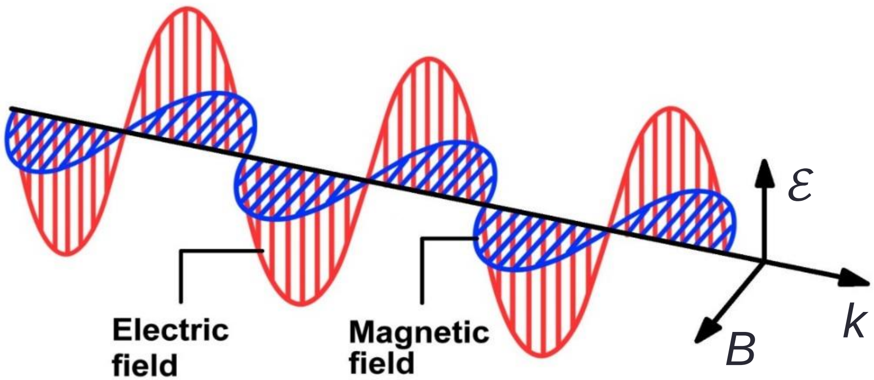
- Intensity of the light wave is proportional to the square of the amplitude of the electric field.
- Square of the wave function for a particle as a probability density for that particle.

Photon and Electromagnetic Wave
电磁波



Photoelectric effect
(1) $E_{photon} = h\nu$

VS



Electromagnetic wave
(2) $E_{light} \propto \mathcal{E}^2$

(1)+(2):
$N_{photon} \propto \mathcal{E}^2$

Light frequency → Energy of a single photon

Light intensity → Number of photons

Summary

- Wave–particle duality
  - Light can behave like particles
  - Electrons can behave like waves
- Wave functions
  - Describes the motion of both light and electrons
  - Its square equals probability
  - Its number of nodes indicates energy

$$E_{\text{photon}} = hv$$

$$p_{\text{photon}} = \frac{h}{\lambda}$$

$$\lambda_{\text{electron}} = \frac{h}{p}$$

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

Quantum number = Number of nodes

Brief history of Early Quantum Mechanics

- **On light**
- 1900 Max Planck: $E_n = nhv$
- 1905 Albert Einstein: $E = mc^2$ $p_{\text{photon}} = \frac{h}{\lambda}$
- 1913 Niels Bohr: The Bohr Model for H

- **On matter**
- 1924 Louis de Broglie: $p = m_e v = \frac{h}{\lambda}$
- 1926 Erwin Schrödinger: Schrödinger Equation
- 1926 Max Born: $P(x) = |\psi(x)|^2$

Next lecture series: The hydrogen atom

Reading: OGC §5.1, YY §2.3