# VE320 – Summer 2024

# Introduction to Semiconductor Devices

Instructor: Yaping Dan （但亚平）
yaping.dan@sjtu.edu.cn

## Chapter 2 Introduction to Quantum Mechanics

# Outline

2.1 $2^{nd}$ order differential equations and waves

2.2 Historic events in developing quantum mechanics

2.3 A case study

2.4 Electrons in infinite quantum well

2.5 Electrons in finite quantum well

2.6 Electrons in an atom

# Outline

**2.1 $2^{nd}$ order differential equations and waves**

2.2 Historic events in developing quantum mechanics

2.3 A case study

2.4 Electrons in infinite quantum well

2.5 Electrons in finite quantum well

2.6 Electrons in an atom

# 2.1 $2^{nd}$ order differential equations and waves

$$\frac{\partial^2 y}{\partial x^2} = k^2 y$$

General solution: $y = Ae^{bx}$

$$\frac{\partial^2 y}{\partial x^2} = -k^2 y$$

General solution: $y = Ae^{bx}$

# 2.1 2nd order differential equations and waves

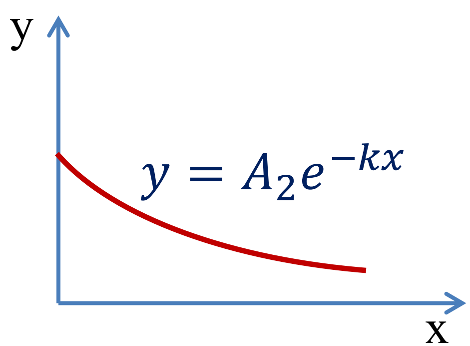
$$\frac{\partial^2 y}{\partial x^2} = k^2 y$$

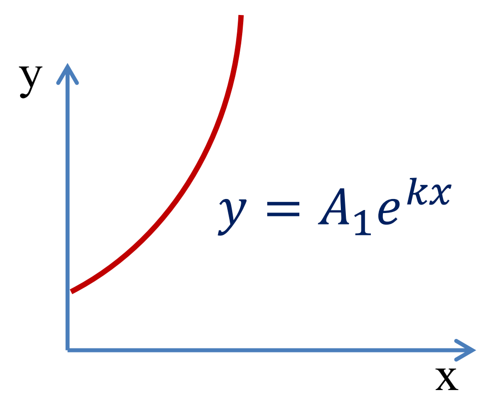
General solution: $y = Ae^{bx}$

Plug into the equation: $b^2 Ae^{bx} = k^2 Ae^{bx}$

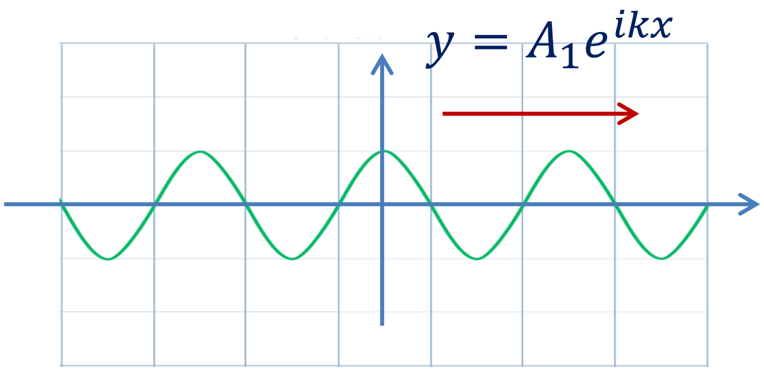
$$\Rightarrow b = \pm k$$

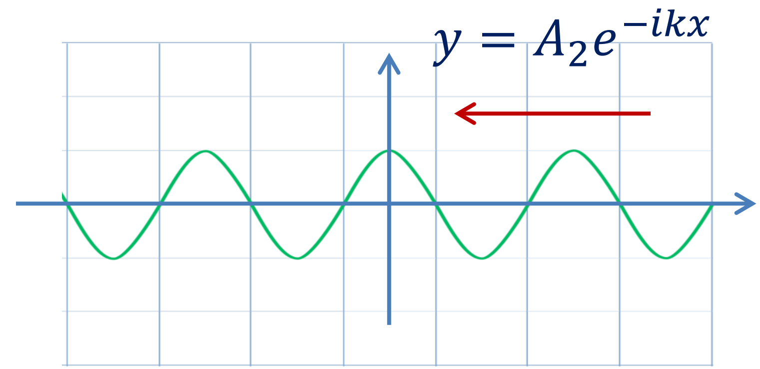
$$\Rightarrow y = A_1 e^{kx} + A_2 e^{-kx}$$



# 2.1 2nd order differential equations and waves




$$\frac{\partial^2 y}{\partial x^2} = -k^2 y$$

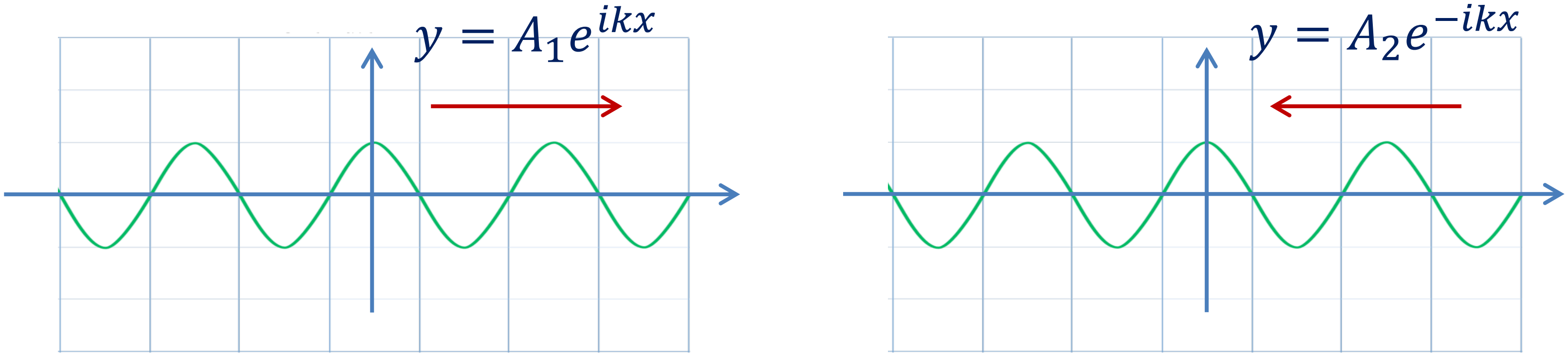
General solution: $y = Ae^{bx}$

Plug into the equation: $b^2 A e^{bx} = -k^2 A e^{bx}$

$$\Rightarrow b = \pm ki$$

$$\Rightarrow y = A_1 e^{ikx} + A_2 e^{-ikx}$$

# 2.1 $2^{nd}$ order differential equations and waves

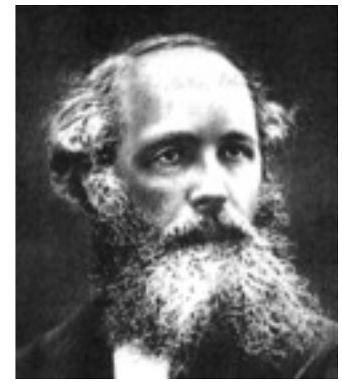



1. Give a wave propagating along x with a wavelength $\lambda_0$, please write the static $2^{nd}$ order differential equation that governs the behavior of this wave.

# 2.1 2nd order differential equations and waves

- Electromagnetic (EM) wave

$$\begin{cases} \nabla \cdot E = 4\pi\rho \\ \nabla \times E = -\dfrac{1}{\sqrt{\mu\varepsilon}}\dfrac{\partial B}{\partial t} \\ \nabla \cdot B = 0 \\ \nabla \times B = \dfrac{4\pi}{c}J + \dfrac{1}{\sqrt{\mu\varepsilon}}\dfrac{\partial E}{\partial t} \end{cases}$$



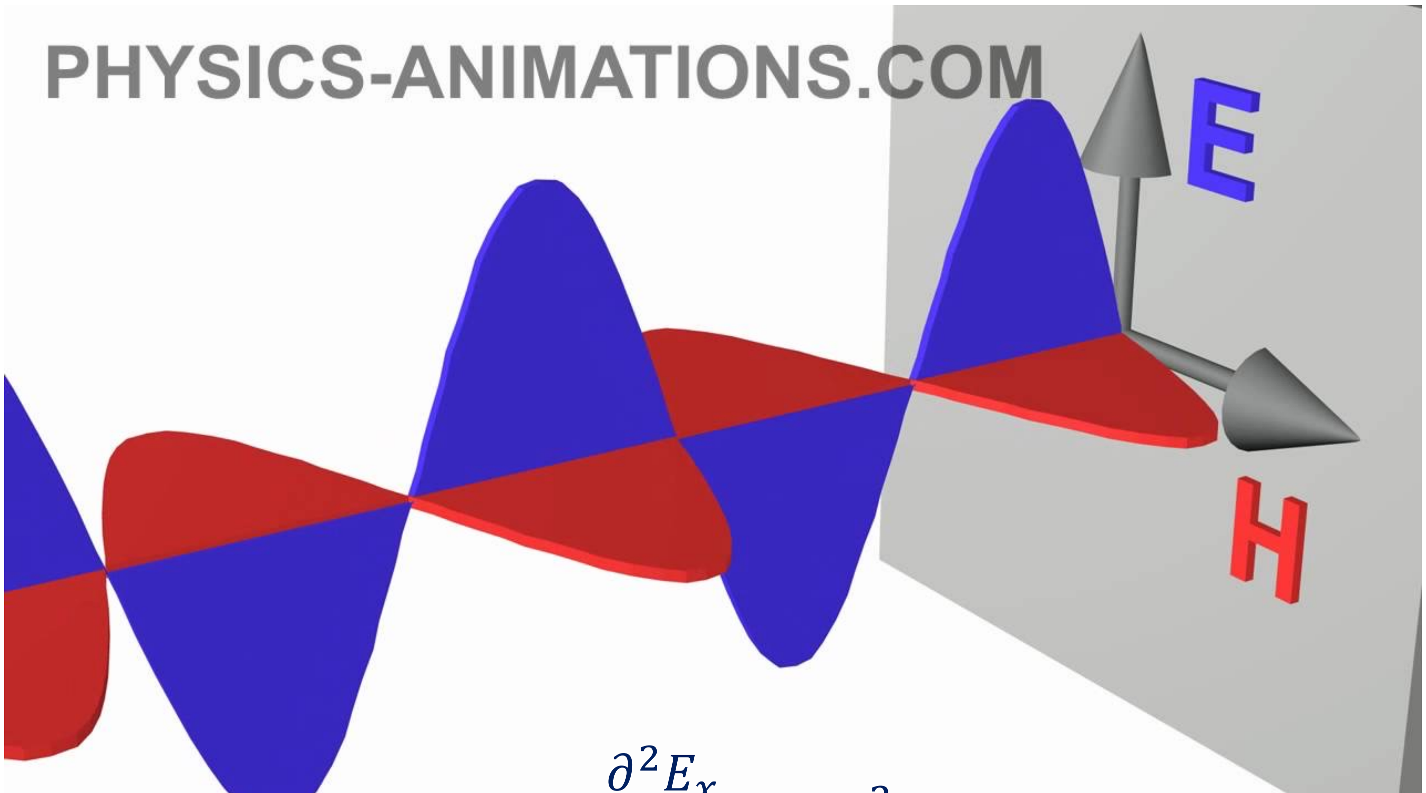
James Maxwell

Static differential equation describing the electromagnetic wave

$$\frac{\partial^2 E_x}{\partial x^2} = -\omega^2\mu\varepsilon E_x = -(\omega\sqrt{\mu\varepsilon})^2 E_x \qquad E_x = E_{x0}e^{-i\omega\sqrt{\mu\varepsilon}x}$$

# 2.1 2nd order differential equations and waves

- Electromagnetic (EM) wave




$$\frac{\partial^2 E_x}{\partial x^2} = -\omega^2 \mu \varepsilon E_x$$

# Outline

2.1 $2^{nd}$ order differential equations and waves

**2.2 Historic events in developing quantum mechanics**

2.3 A case study

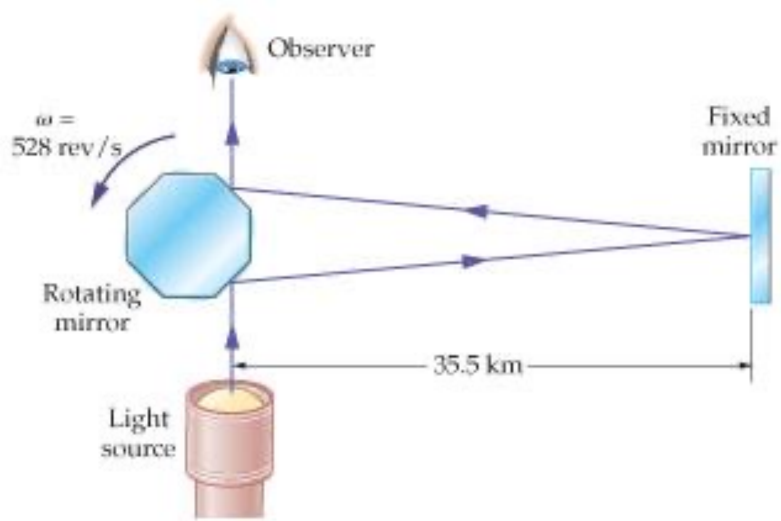
2.4 Electrons in infinite quantum well

2.5 Electrons in finite quantum well

2.6 Electrons in an atom

# 2.2 Historic events in developing quantum mechanics

① Speed of light in 1862 $v = 2.98 \times 10^8 m/s$



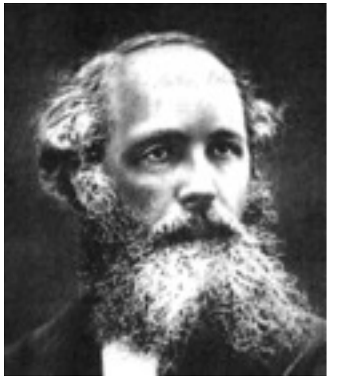

Rotation mirror

Leon Foucault

# 2.2 Historic events in developing quantum mechanics

② Maxwell Equations in the year 1865

$$\begin{cases} \nabla \cdot E = 4\pi\rho \\ \nabla \times E = -\dfrac{1}{\sqrt{\mu\varepsilon}}\dfrac{\partial B}{\partial t} \\ \nabla \cdot B = 0 \\ \nabla \times B = \dfrac{4\pi}{c}J + \dfrac{1}{\sqrt{\mu\varepsilon}}\dfrac{\partial E}{\partial t} \end{cases}$$



James Maxwell

Static differential equation describing the electromagnetic wave

$$\frac{\partial^2 E_x}{\partial x^2} = -\omega^2 \mu\varepsilon E_x$$

$$E_x = E_{x0} e^{-i\omega\sqrt{\mu\varepsilon}x}$$

Light is an electromagnetic wave!

$$v = \frac{1}{\sqrt{\mu\varepsilon}} = 2.99\times 10^8 m/s$$

# 2.2 Historic events in developing quantum mechanics

③ Light wave-particle duality in 1905

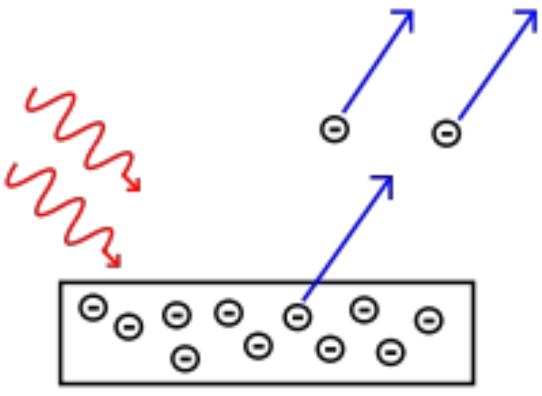
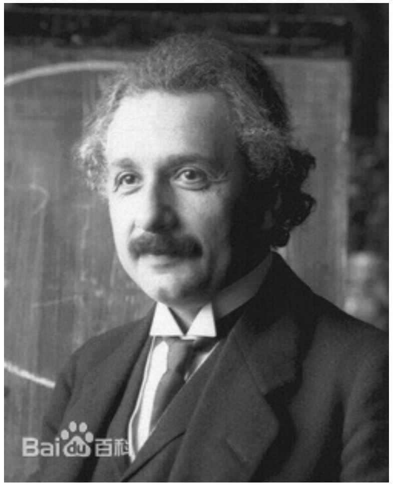


Photo-electric experiment

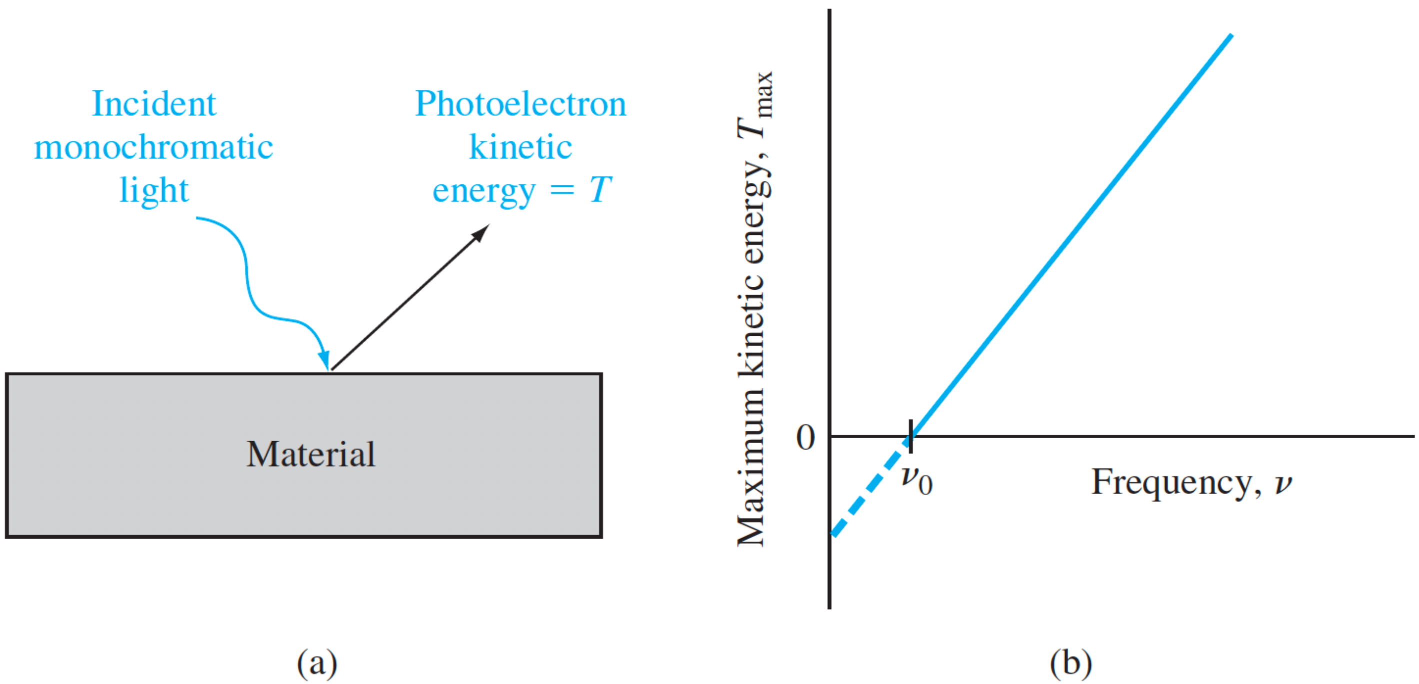



Albert Einstein
Nobel Prize 1921

- ❑ Light frequency higher than a certain frequency → election ejection
- ❑ Not a function of light intensity

# 2.2 Historic events in developing quantum mechanics

## ③ Light wave-particle duality in 1905




- ❑ Light wave is a particle: $hv = K_{max} + W_c$

# 2.2 Historic events in developing quantum mechanics

③ Light wave-particle duality in 1905

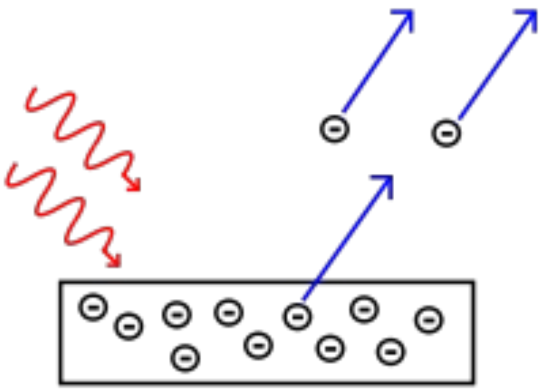
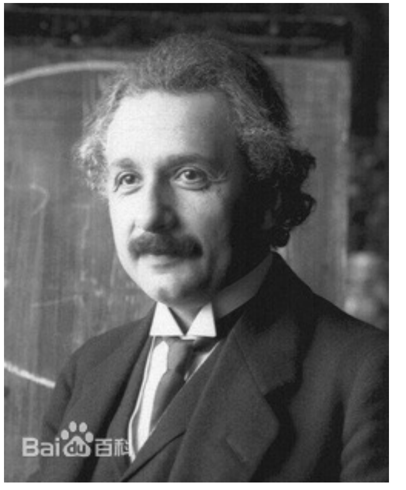


Photo-electric experiment



Albert Einstein
Nobel Prize 1921

$$E = h\text{v} = \hbar\omega$$

$$E = mc^2$$

$$\text{p} = mc = \frac{E}{c} = \frac{h\text{v}}{c} = \frac{h}{\lambda} = \hbar k$$

Light is a particle!

$$k = \frac{2\pi}{\lambda}$$

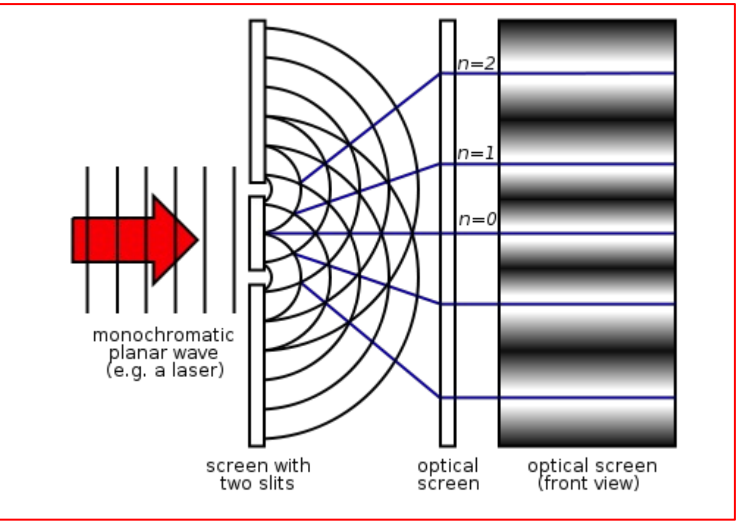
# 2.2 Historic events in developing quantum mechanics

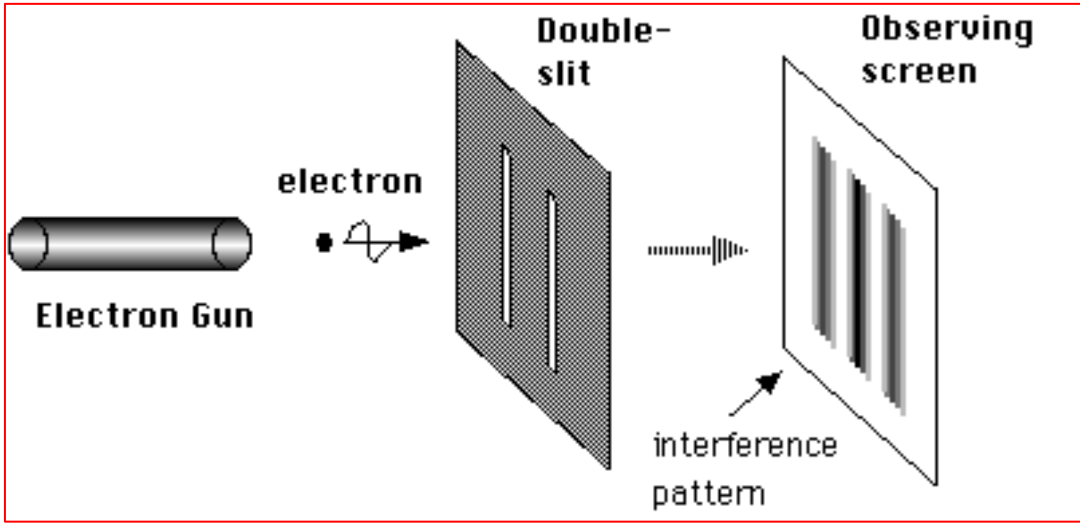
④ Matter wave hypothesis in 1924

Louis Victor de Broglie
Nobel Prize 1929

# 2.2 Historic events in developing quantum mechanics

④ Matter wave hypothesis in 1924



# Outline

2.1 $2^{nd}$ order differential equations and waves

2.2 Historic events in developing quantum mechanics

**2.3 A case study**

2.4 Electrons in infinite quantum well

2.5 Electrons in finite quantum well

2.6 Electrons in an atom

# 2.3 A case study

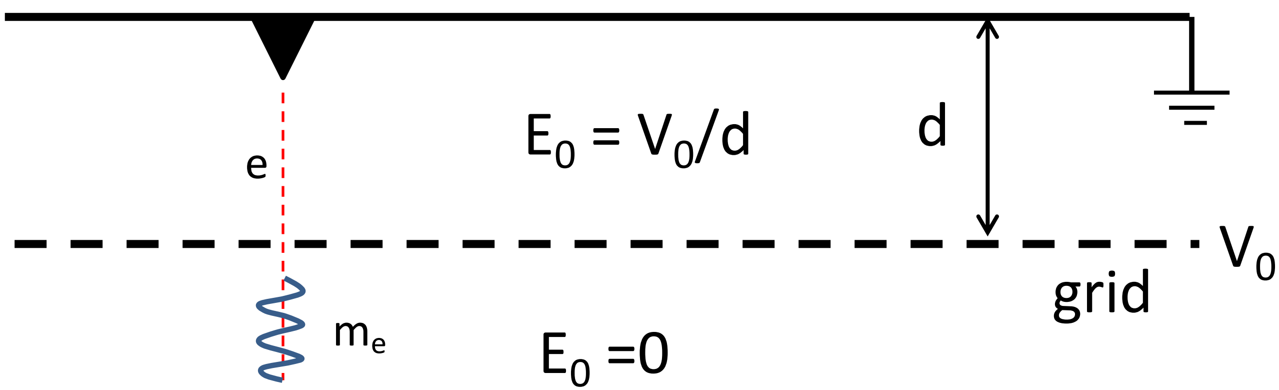
$$\frac{\partial^2 y}{\partial x^2} = -k^2 y$$

- Maxwell Equation in the year 1865
- Light wave-particle duality in 1905
- Matter wave hypothesis in 1924

$$E = \frac{1}{2}mv^2 \qquad E = h\text{v} = \hbar\omega$$

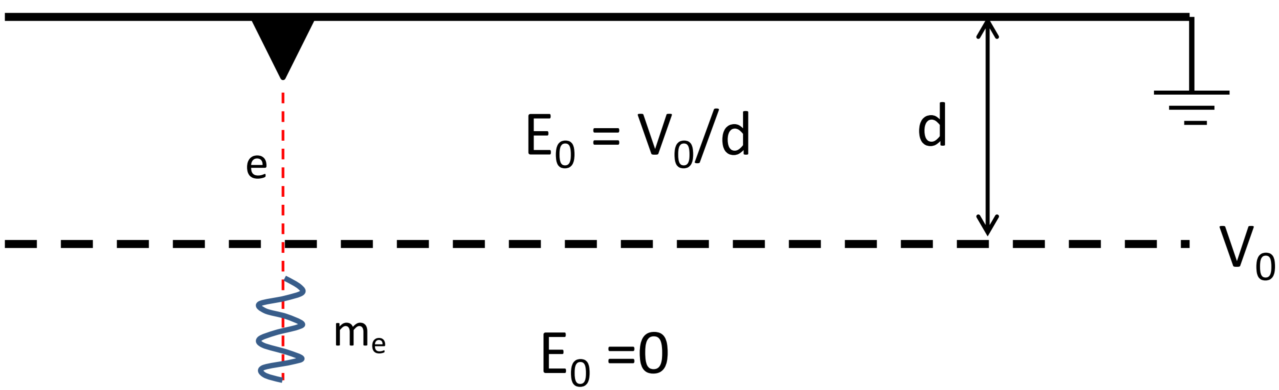
$$\text{p} = mv \qquad \text{p} = \frac{h}{\lambda} = \hbar k$$

Quiz #1:




Can you find a differential equation that governs the wave behavior of electrons?

# 2.3 A case study




Can you find a differential equation that governs the wave behavior of electrons?

# 2.3 A case study

# Outline

2.1 $2^{nd}$ order differential equations and waves

2.2 Historic events in developing quantum mechanics

2.3 A case study

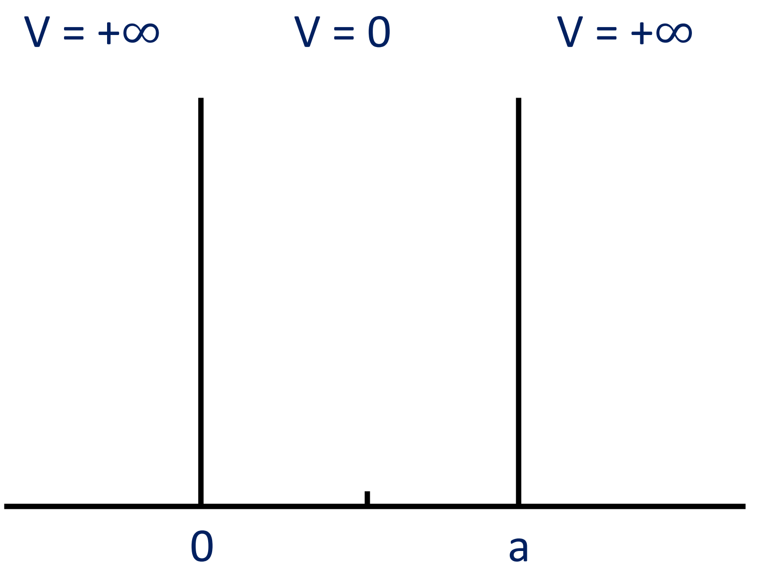
**2.4 Electrons in infinite quantum well**

2.5 Electrons in finite quantum well

2.6 Electrons in an atom

# 2.4 Electrons in Infinite Quantum Well

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




Conditions:

$for\ x \le 0, x \ge a$

$$V(x) = +\infty;$$

$for\ 0 < x < a$

$$V(x) = 0$$

# 2.4 Electrons in Infinite Quantum Well

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

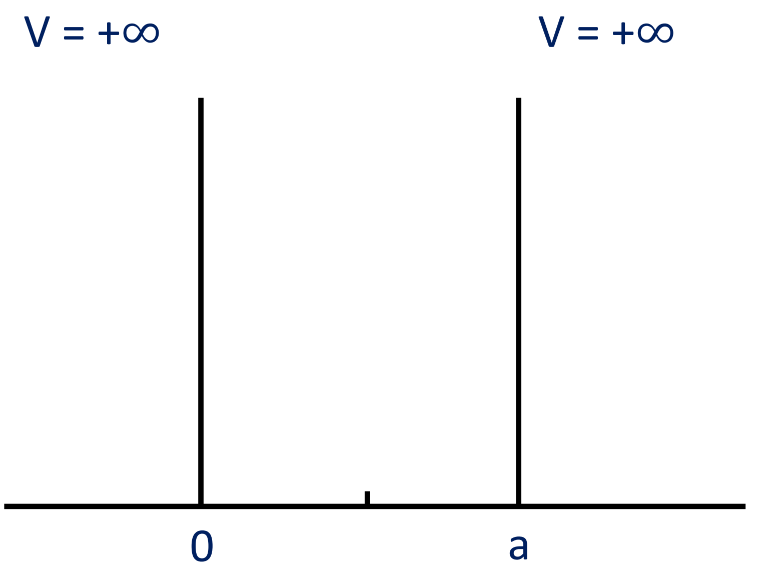
Conditions:

$for\ x \le 0, x \ge a$

$$V(x)=+\infty; \Rightarrow \Psi(x)=0$$

$for\ 0 < x < a$

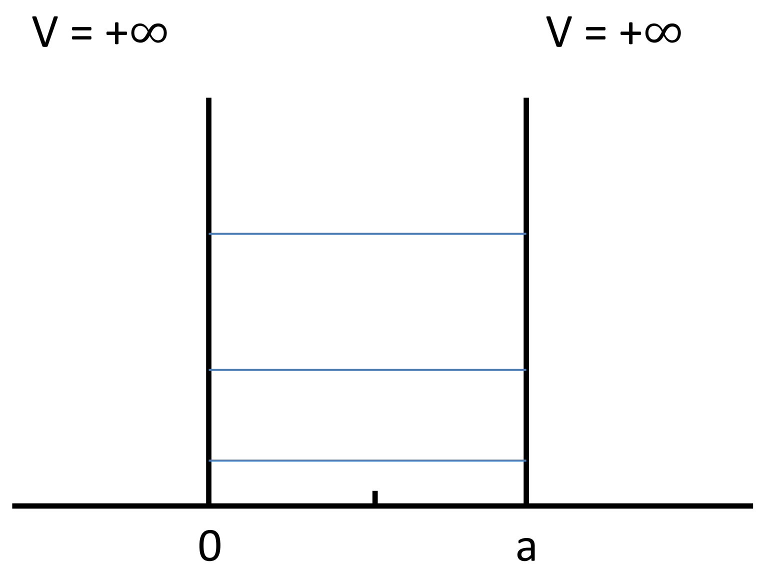
$$V(x)=0$$



# 2.4 Electrons in Infinite Quantum Well

# 2.4 Electrons in Infinite Quantum Well

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




Conditions:

$$for\ x \le 0, x \ge a$$

$$V(x)=+\infty;\ \Psi(x)=0$$

$$for\ 0<x<a$$

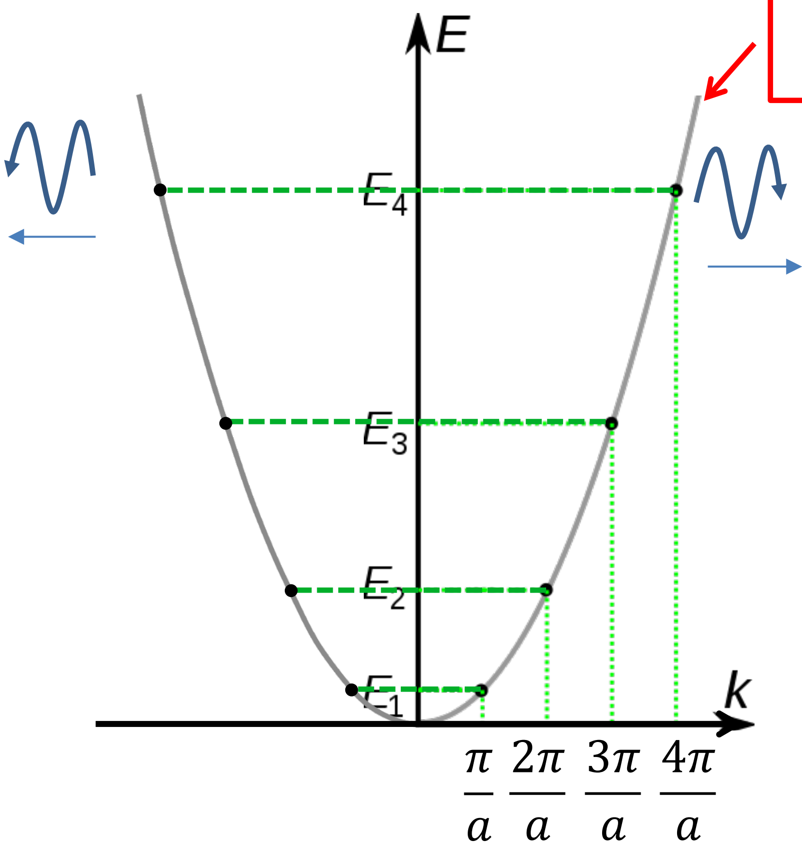
$$V(x)=0$$

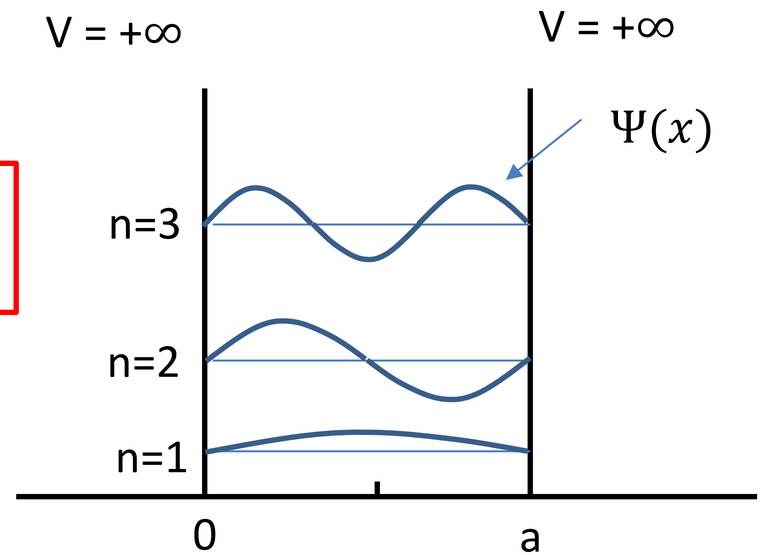
$$\mathrm{E}=\frac{k^2\hbar^2}{2m}=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

# 2.4 Electrons in Infinite Quantum Well

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

$$\boxed{\mathrm{E}=\frac{k^2\hbar^2}{2m}}$$

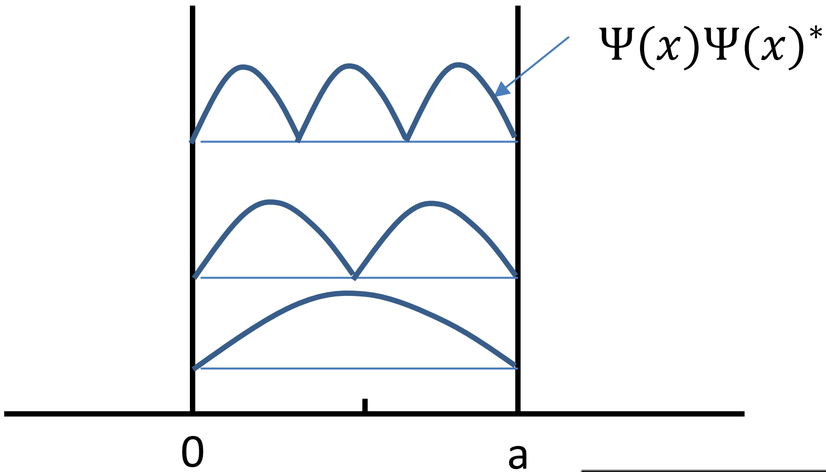


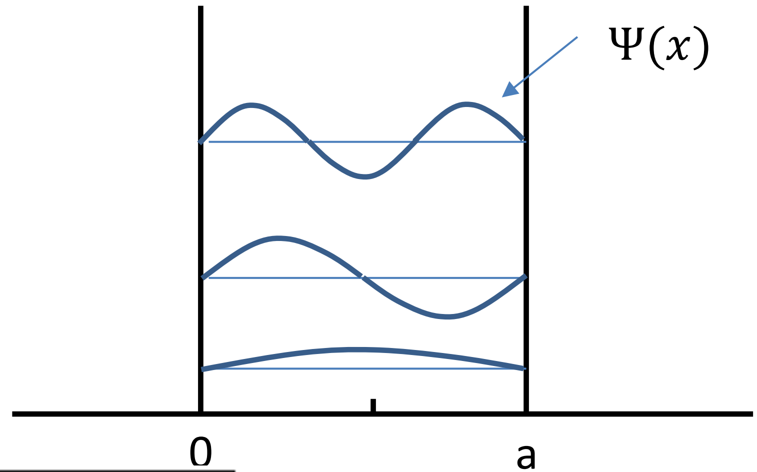



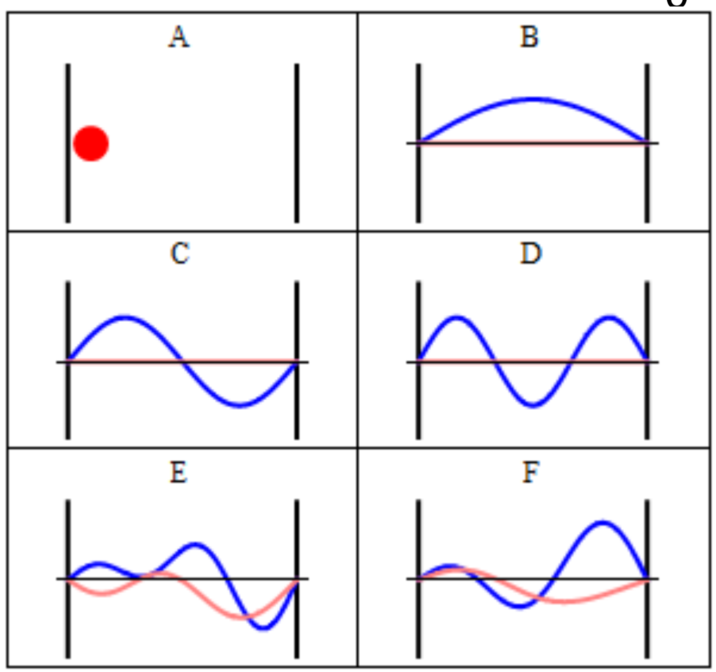

$$\mathrm{E}=\frac{k^2\hbar^2}{2m}=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

$$k=\frac{n\pi}{a}\qquad n=0,\pm1,\pm2,\ldots$$

# 2.4 Electrons in Infinite Quantum Well

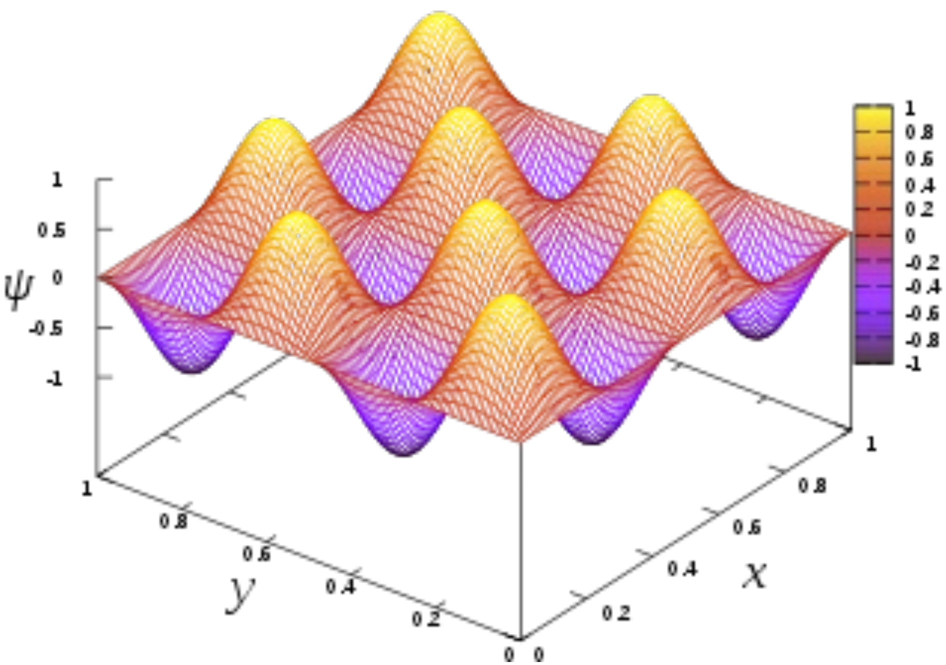


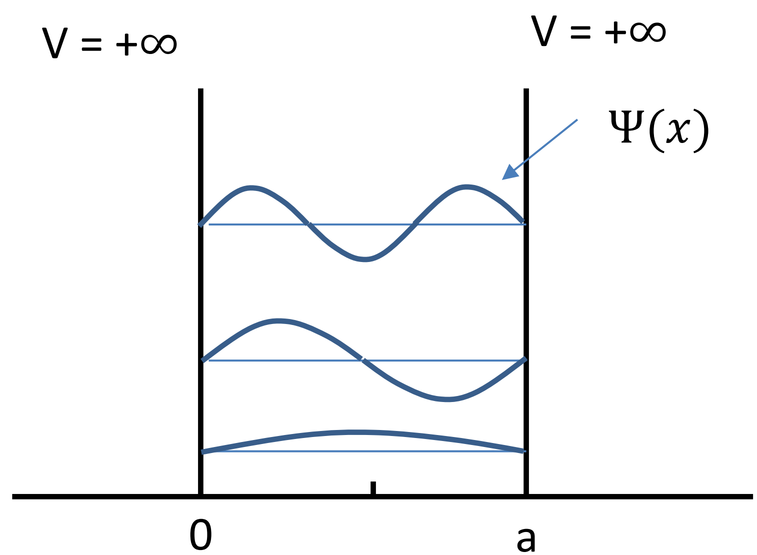



# 2.4 Electrons in Infinite Quantum Well

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




2-dimentional Quantum well




$$\mathrm{E}=\frac{k^2\hbar^2}{2m}=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

# Outline

2.1 $2^{nd}$ order differential equations and waves

2.2 Historic events in developing quantum mechanics

2.3 A case study

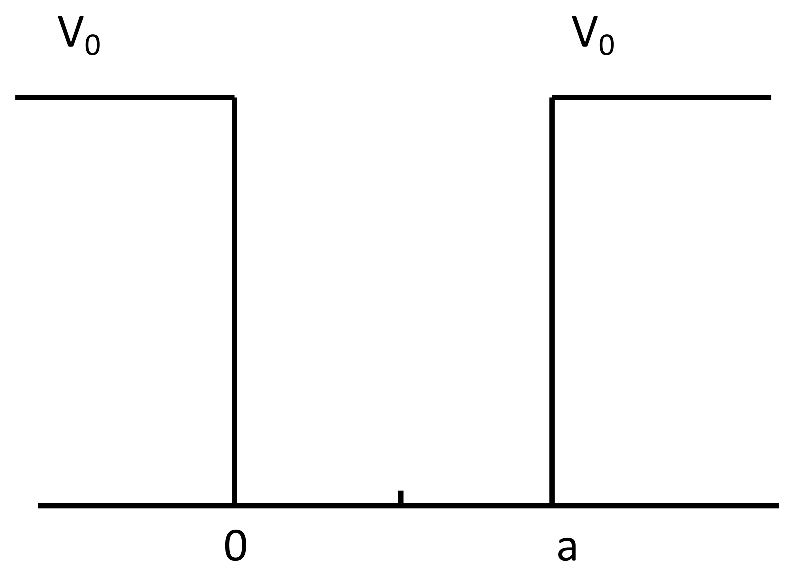
2.4 Electrons in infinite quantum well

**2.5 Electrons in finite quantum well**

2.6 Electrons in an atom

# 2.5 Electrons in Finite Quantum Well

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




Conditions:

$for\ x \le 0, x \ge a$

$$V(x)=V_0;$$

$for\ 0<x<a$

$$V(x)=0$$

# 2.5 Electrons in Finite Quantum Well

# 2.5 Electrons in Finite Quantum Well

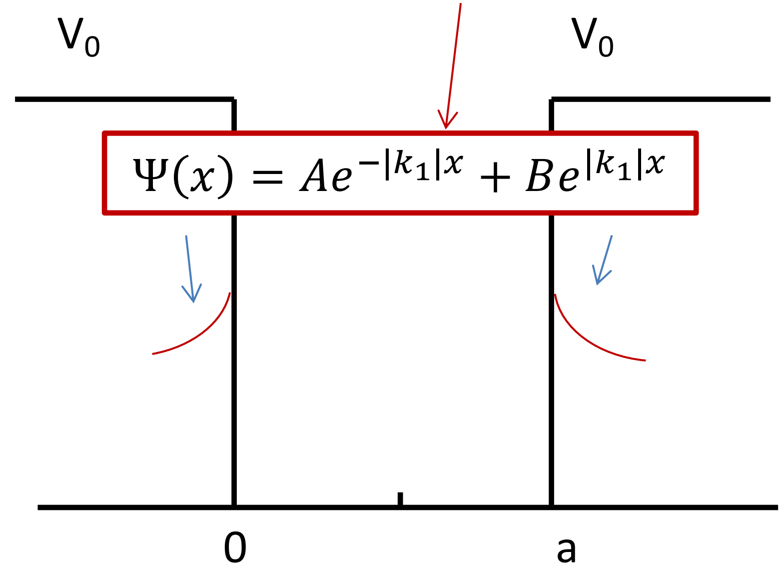
If E < $V_0$ $\quad k_1 = i\sqrt{\dfrac{2m(V_0 - E)}{\hbar^2}}$

Boundary Conditions:

$$\Psi(x)|_{x=a,0} \ \ continous$$

$$\Psi'(x)|_{x=a,0} \ \ continous$$

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1$$




$$\boxed{\Psi(x) = Ae^{-|k_1|x} + Be^{|k_1|x}}$$

$for\ x < 0, x > a$

$$\boxed{\Psi(x) = Ae^{-ik_1x} + Be^{ik_1x}} \qquad k_1 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

$for\ 0 \le x \le a$

$$\boxed{\Psi(x) = Ce^{-ik_2x} + De^{ik_2x}} \qquad k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$

# 2.5 Electrons in Finite Quantum Well

Boundary Conditions:

$$\Psi(x)|_{x=a,0} \ \ continous$$

$$\Psi'(x)|_{x=a,0} \ \ continous$$

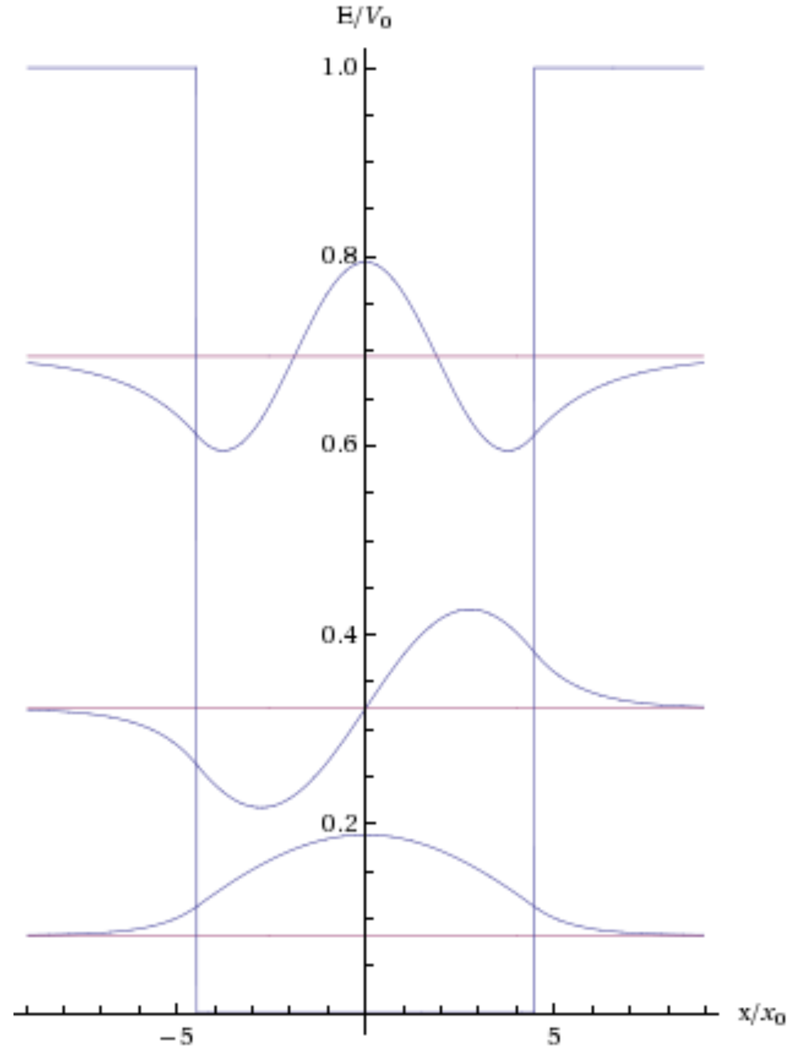
$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1$$

$$for\, x < 0, x > a$$

$$\boxed{\Psi(r) = Ae^{-ik_1x} + Be^{ik_1x}}$$

$$for\, 0 \leq x \leq a$$

$$\boxed{\Psi(r) = Ce^{-ik_2x} + De^{ik_2x}}$$



# Outline

2.1 $2^{nd}$ order differential equations and waves

2.2 Historic events in developing quantum mechanics

2.3 A case study

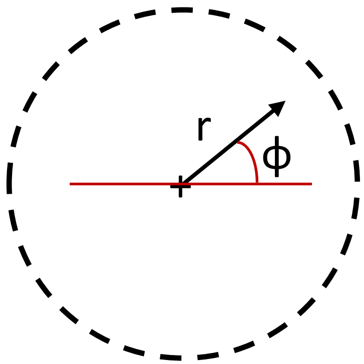
2.4 Electrons in infinite quantum well

2.5 Electrons in finite quantum well

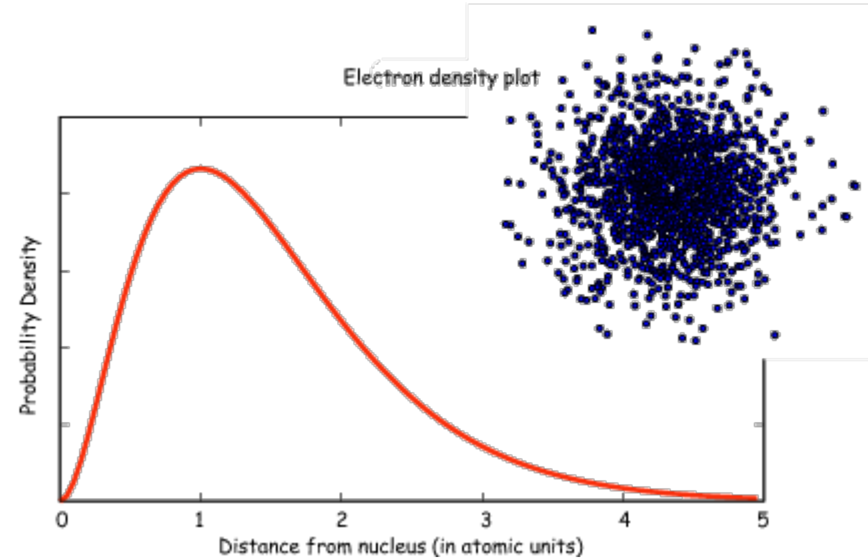
**2.6 Electrons in an atom**

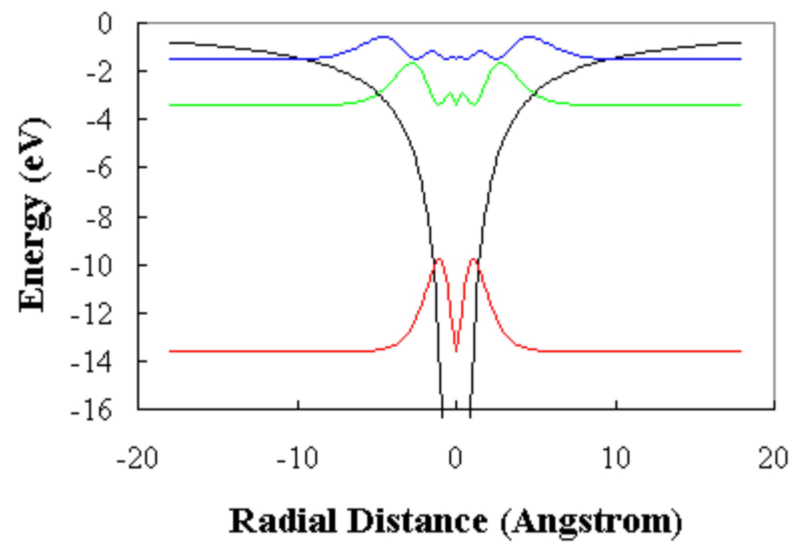
# 2.6 Electrons in an Atom

- 2D



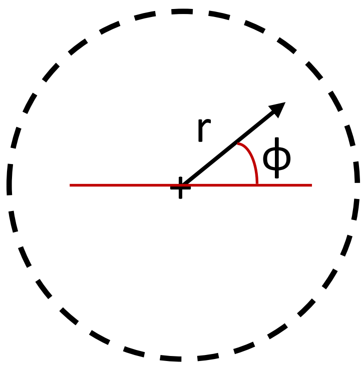

Periodic boundary conditions

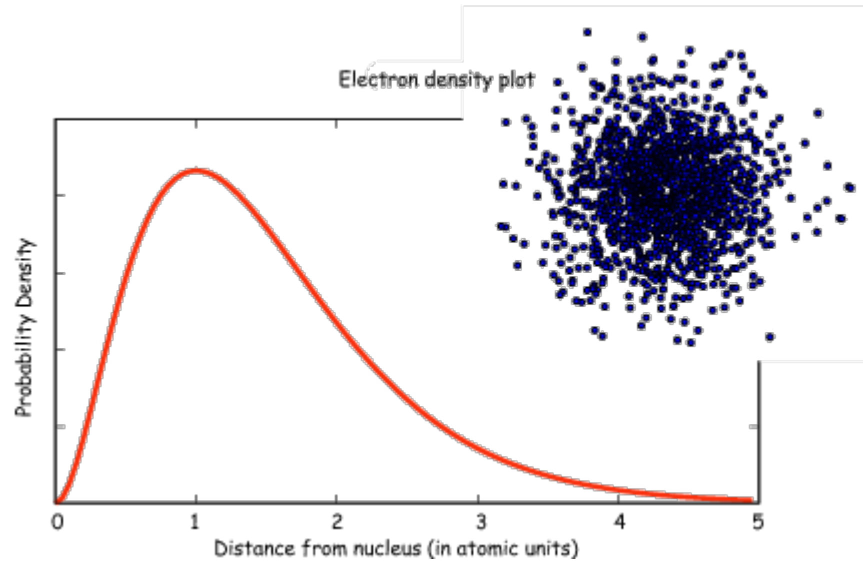


# 2.6 Electrons in an Atom

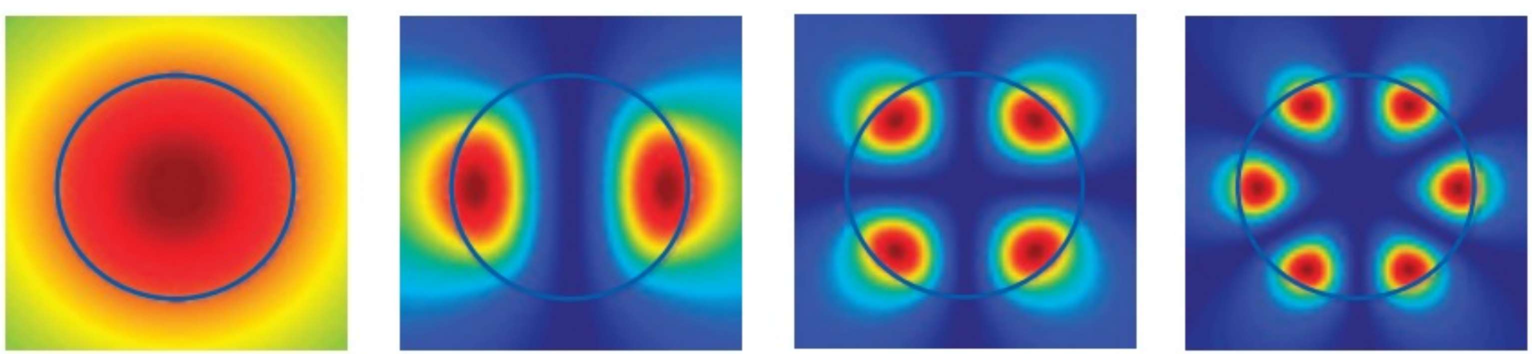
- 2D



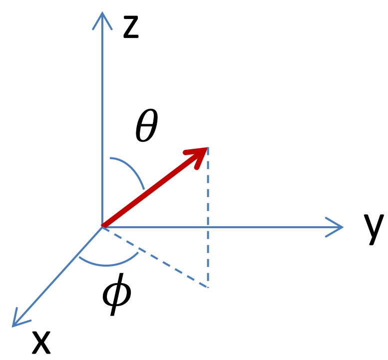

Periodic boundary conditions

$f(r, \phi)$



# 2.6 Electrons in an Atom

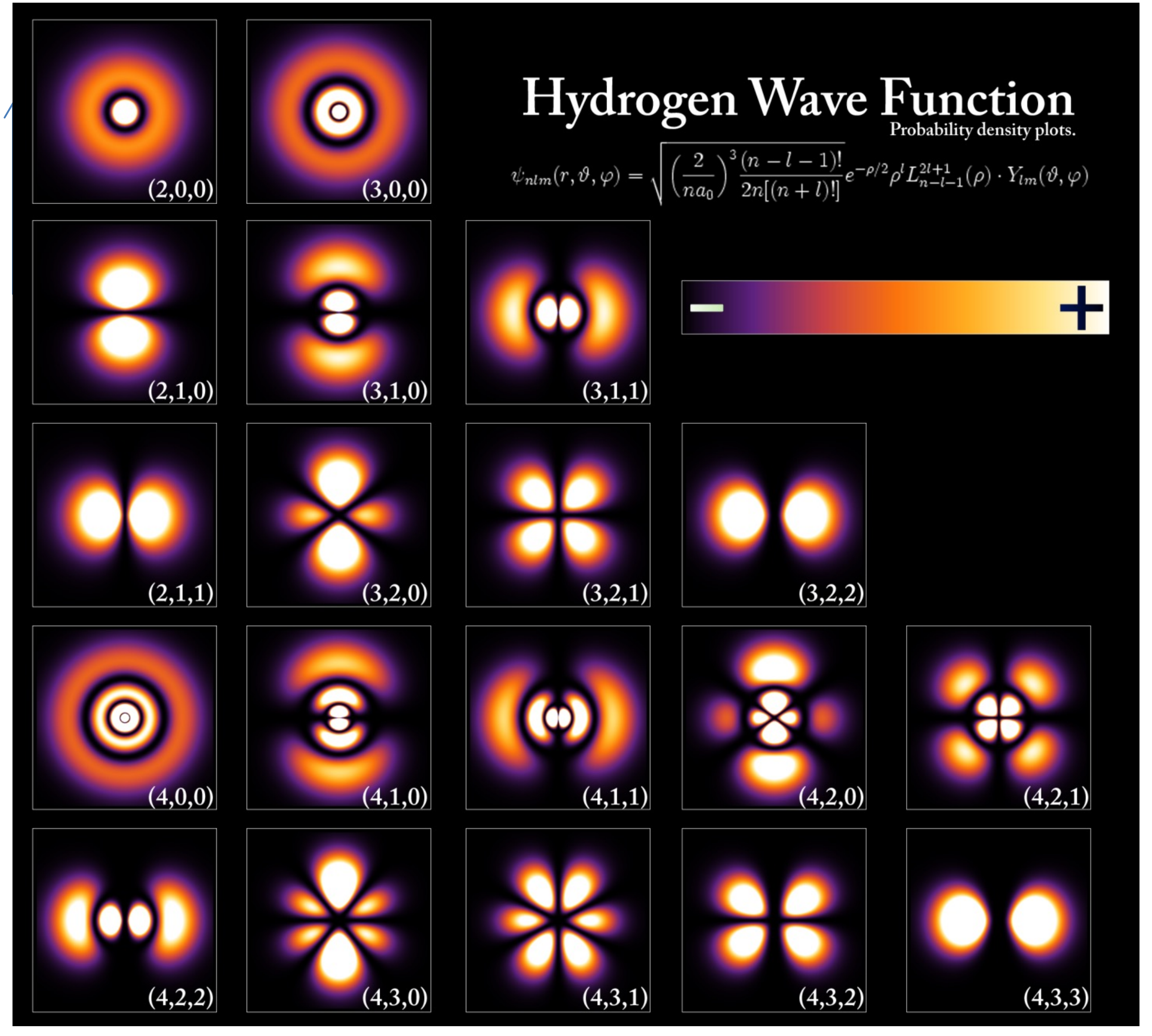
- 3D




$$\Psi_{r,\theta,\phi} = R_n^l(r)Y_l^m(\phi,\theta)$$

# 2.6 Electrons in an Atom

- 3D




$3s^2 3p^6 3d^6$

$2s^2 2p^6$

$1s^2$

# 2.6 Electrons in an Atom

- 3D

**Table 2.1** | Initial portion of the periodic table

| Element | Notation | $n$ | $l$ | $m$ | $s$ |
|---|---|---|---|---|---|
| Hydrogen | $1s^1$ | 1 | 0 | 0 | $+\frac{1}{2}$ or $-\frac{1}{2}$ |
| Helium | $1s^2$ | 1 | 0 | 0 | $+\frac{1}{2}$ and $-\frac{1}{2}$ |
| Lithium | $1s^2 2s^1$ | 2 | 0 | 0 | $+\frac{1}{2}$ or $-\frac{1}{2}$ |
| Beryllium | $1s^2 2s^2$ | 2 | 0 | 0 | $+\frac{1}{2}$ and $-\frac{1}{2}$ |
| Boron | $1s^2 2s^2 2p^1$ | 2 | 1 | | |
| Carbon | $1s^2 2s^2 2p^2$ | 2 | 1 | | |
| Nitrogen | $1s^2 2s^2 2p^3$ | 2 | 1 | | $m = 0, -1, +1$ |
| Oxygen | $1s^2 2s^2 2p^4$ | 2 | 1 | | $s = +\frac{1}{2}, -\frac{1}{2}$ |
| Fluorine | $1s^2 2s^2 2p^5$ | 2 | 1 | | |
| Neon | $1s^2 2s^2 2p^6$ | 2 | 1 | | |