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**VE320 – Summer 2022**

**Introduction to Semiconductor Devices**

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**Chapter 2 Introduction to Quantum Mechanics**

# Outline

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2.1 2<sup>nd</sup> 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

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**2.1 2<sup>nd</sup> 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<sup>nd</sup> order differential equations and waves

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

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 2<sup>nd</sup> order differential equations and waves

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

$$\Rightarrow b = \pm k$$

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

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

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

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

$$\Rightarrow b = \pm ki$$

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

## 2.1 2<sup>nd</sup> order differential equations and waves

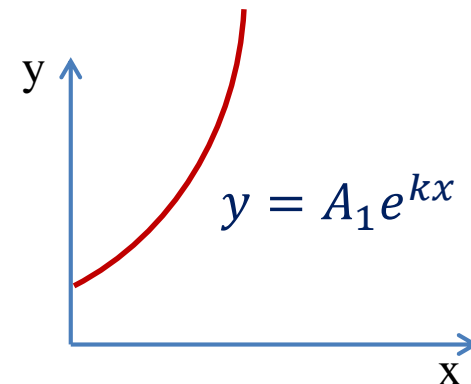
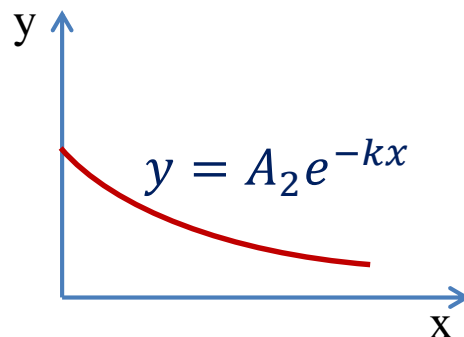
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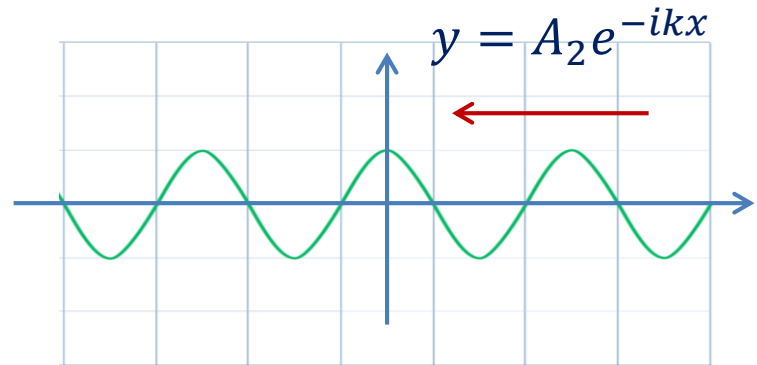
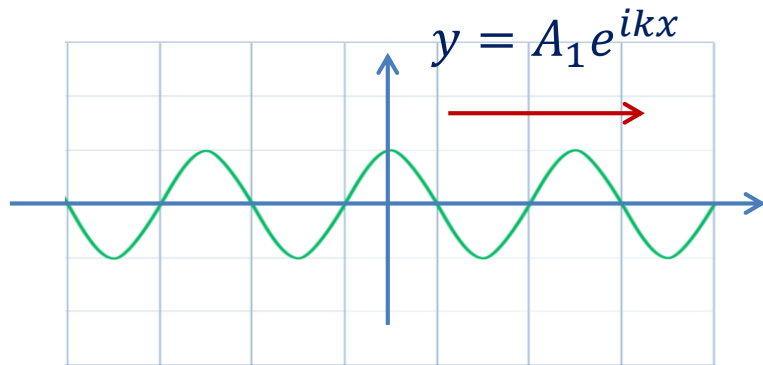
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## 2.1 2<sup>nd</sup> order differential equations and waves



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

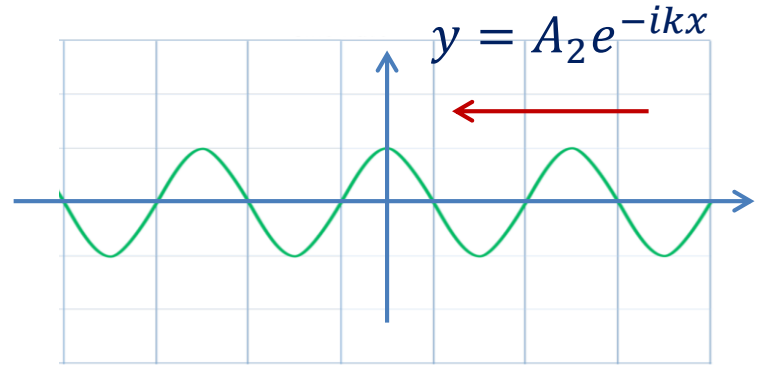
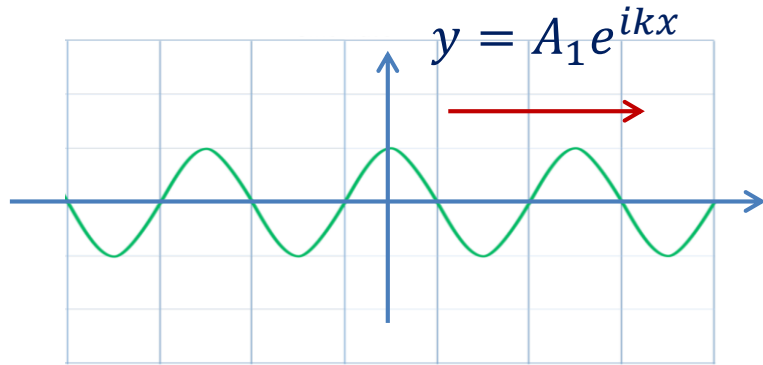
General solution:  $y = Ae^{bx}$

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

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

## 2.1 2<sup>nd</sup> order differential equations and waves



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



## 2.1 2<sup>nd</sup> order differential equations and waves

- Electromagnetic (EM) wave

$$\left\{ \begin{array}{l} \nabla \cdot E = 4\pi\rho \\ \nabla \times E = -\frac{1}{\sqrt{\mu\varepsilon}} \frac{\partial B}{\partial t} \\ \nabla \cdot B = 0 \\ \nabla \times B = \frac{4\pi}{c} J + \frac{1}{\sqrt{\mu\varepsilon}} \frac{\partial E}{\partial t} \end{array} \right.$$



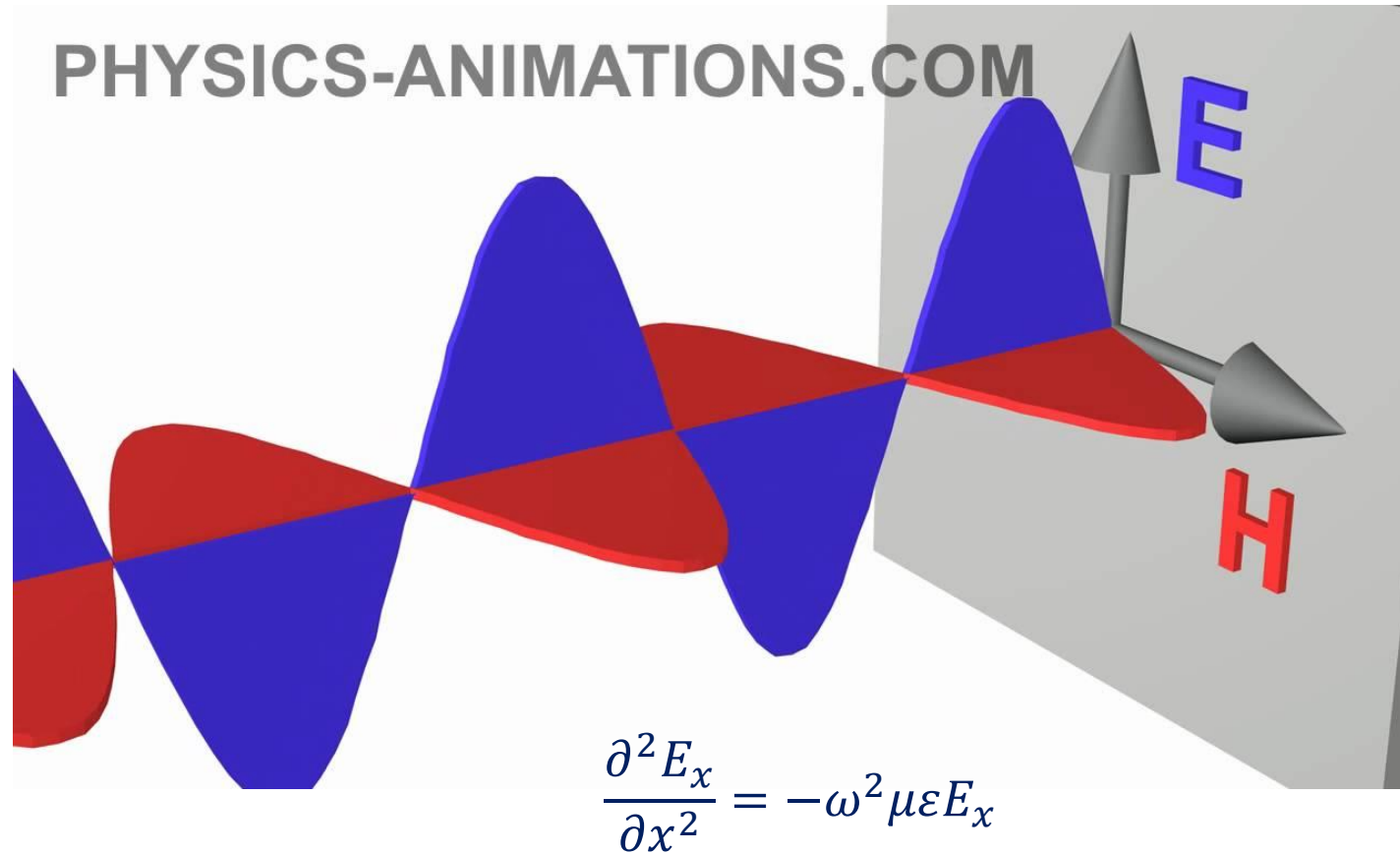
James Maxwell

Static differential equation describing the electromagnetic wave

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

## 2.1 2<sup>nd</sup> order differential equations and waves

- Electromagnetic (EM) wave



# Outline

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2.1 2<sup>nd</sup> order differential equations and waves

**2.2 Historic events in developing quantum mechanics**

2.3 A case study

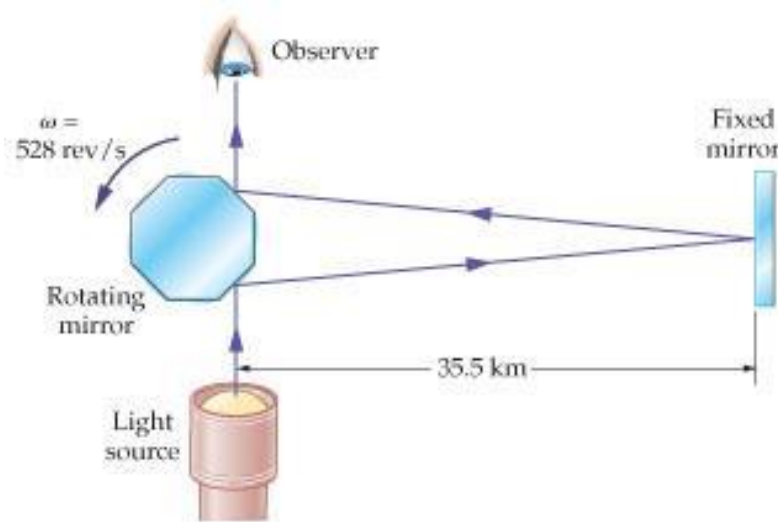
2.4 Electrons in infinite quantum well

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  $v = 2.98 \times 10^8 \text{ m/s}$



Rotation mirror



Leon Foucault

## 2.2 Historic events in developing quantum mechanics

### ② Maxwell Equations in the year 1865

$$\left\{ \begin{array}{l} \nabla \cdot E = 4\pi\rho \\ \nabla \times E = -\frac{1}{\sqrt{\mu\varepsilon}} \frac{\partial B}{\partial t} \\ \nabla \cdot B = 0 \\ \nabla \times B = \frac{4\pi}{c} J + \frac{1}{\sqrt{\mu\varepsilon}} \frac{\partial E}{\partial t} \end{array} \right.$$



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!

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

## 2.2 Historic events in developing quantum mechanics

### ③ Light wave-particle duality in 1905

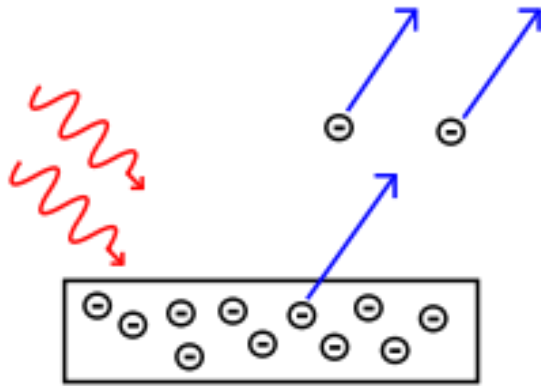
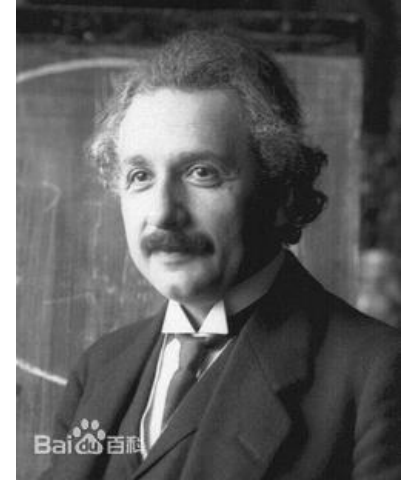


Photo-electric experiment

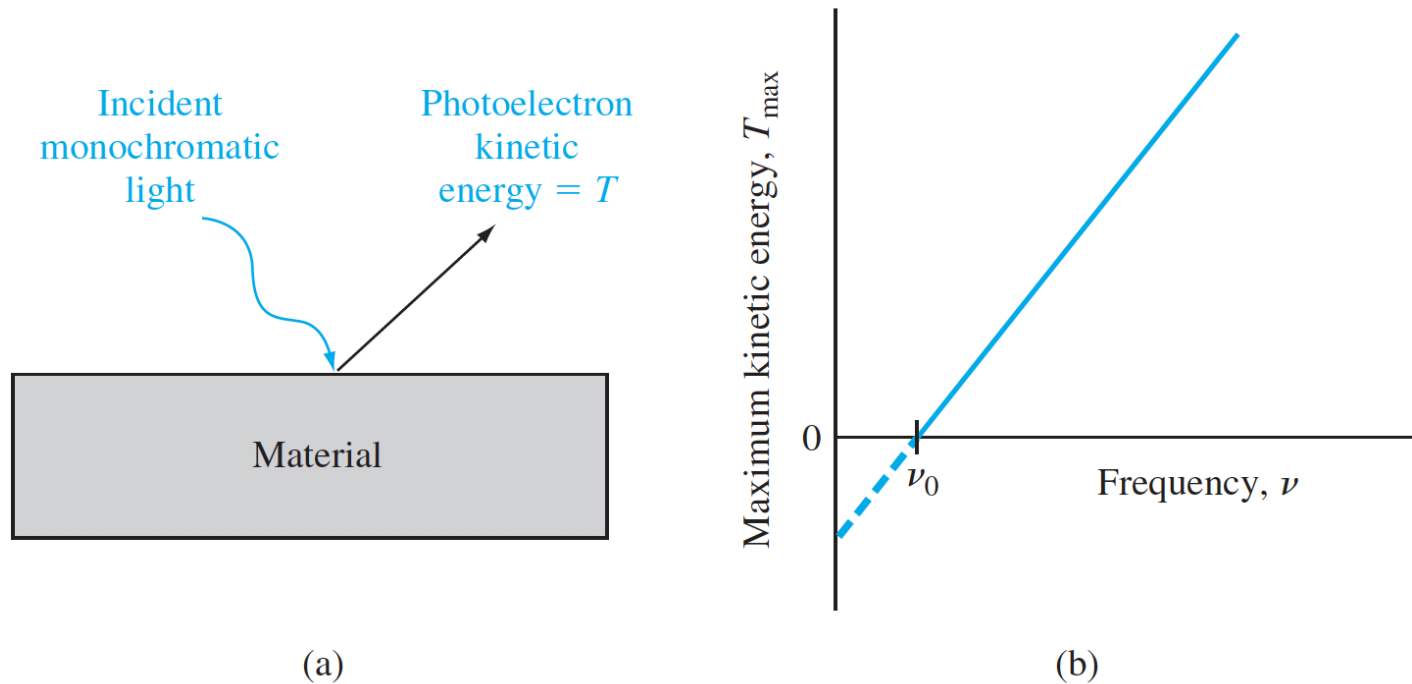


Albert Einstein  
Nobel Prize 1921

- ☐ Light frequency higher than a certain frequency  $\rightarrow$  electron 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:  $h\nu = K_{\max} + W_c$

## 2.2 Historic events in developing quantum mechanics

### ③ Light wave-particle duality in 1905

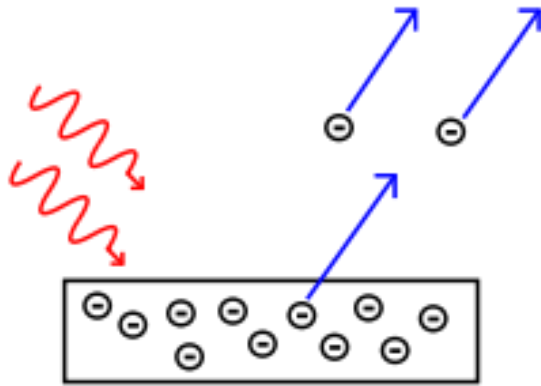
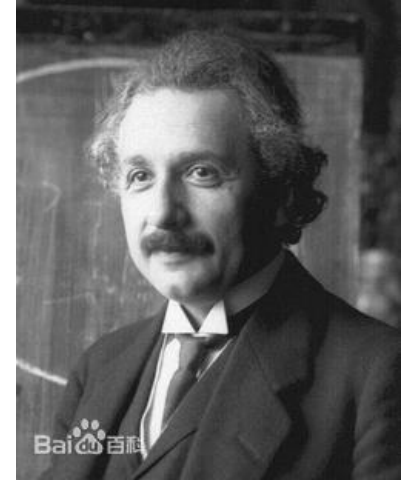


Photo-electric experiment



Albert Einstein  
Nobel Prize 1921

$$E = h\nu = \hbar\omega$$

$$E = mc^2$$

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

Light is a particle!

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



## 2.2 Historic events in developing quantum mechanics

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### ④ Matter wave hypothesis in 1924

$$E = \frac{1}{2}mv^2$$

$$p = mv$$

Matter particle

$$E = h\nu = \hbar\omega$$

$$p = \frac{h}{\lambda} = \hbar k$$

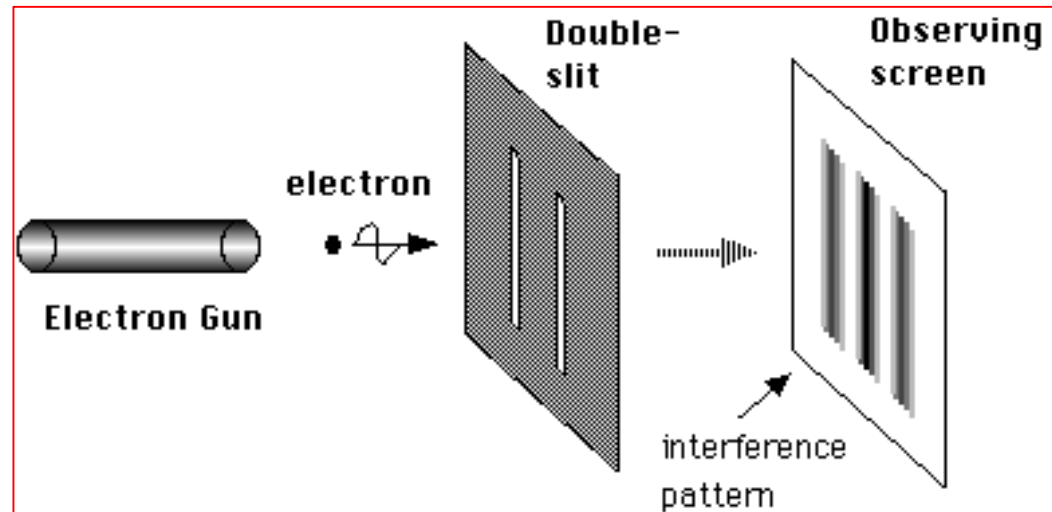
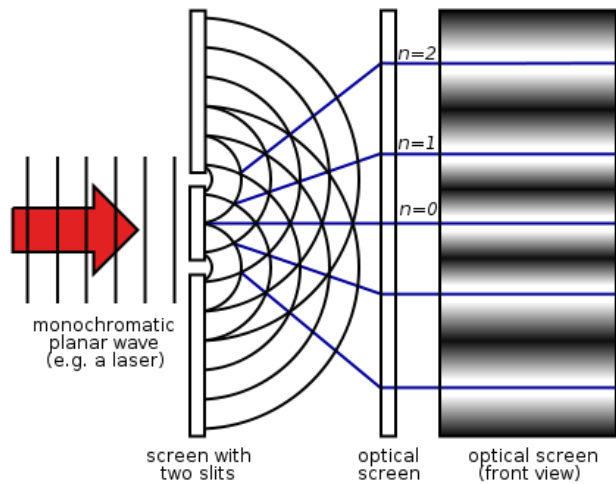
Wave- particle



Louis Victor de Broglie  
Nobel Prize 1929

## 2.2 Historic events in developing quantum mechanics

### ④ Matter wave hypothesis in 1924



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## 2.3 A case study

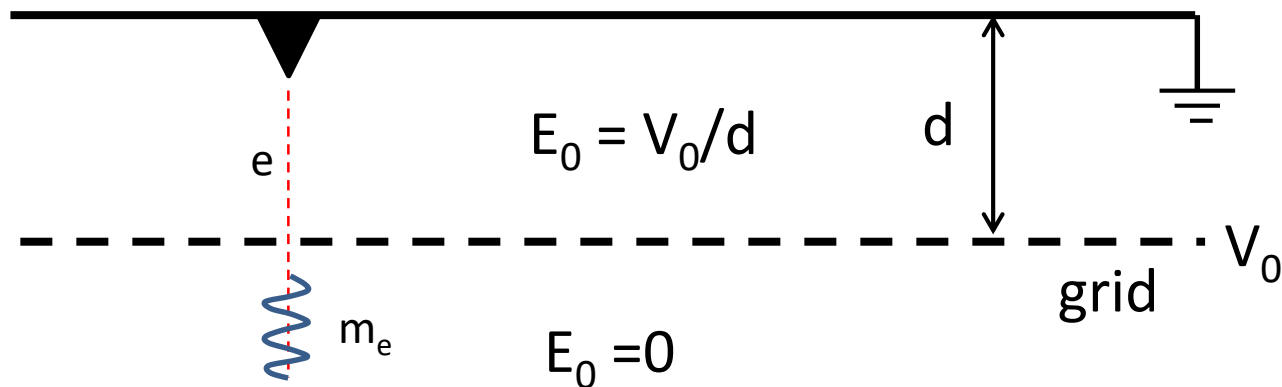
- Maxwell Equation in the year 1865
- Light wave-particle duality in 1905
- Matter wave hypothesis in 1924

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

$$E = \frac{1}{2} m v^2 \quad E = h\nu = \hbar\omega$$

$$p = m v \quad p = \frac{h}{\lambda} = \hbar k$$

Quiz #1:



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

## 2.3 A case study

$$E = qV_0 = \frac{1}{2}mv^2$$

$$p = mv$$

$$E = h\nu = \hbar\omega$$

$$p = \frac{h}{\lambda} = \hbar k$$

$$v = \sqrt{\frac{2qV_0}{m}}$$

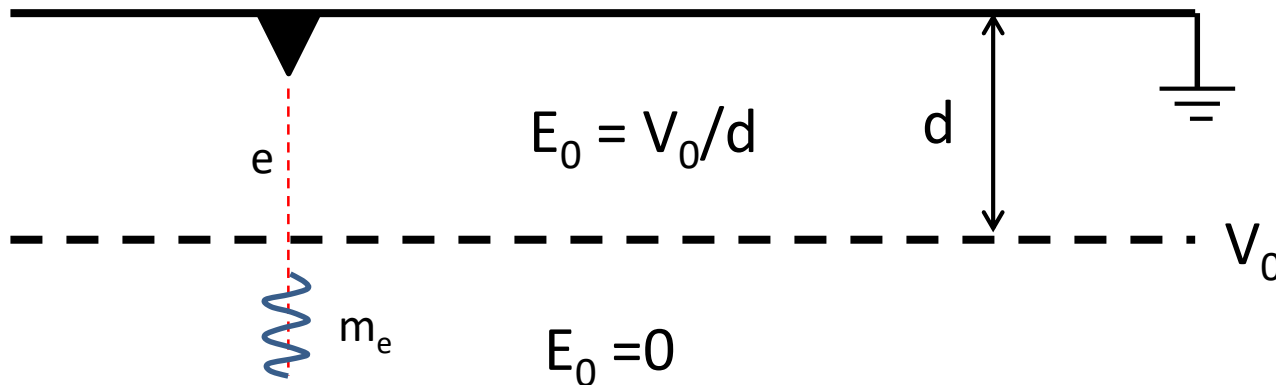
$$k = \frac{m}{\hbar} v = \sqrt{\frac{2mqV_0}{\hbar^2}}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 \Psi = -\frac{2mqV_0}{\hbar^2} \Psi$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$

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

# Schrodinger Equation !



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

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## 2.4 Electrons in Infinite Quantum Well

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

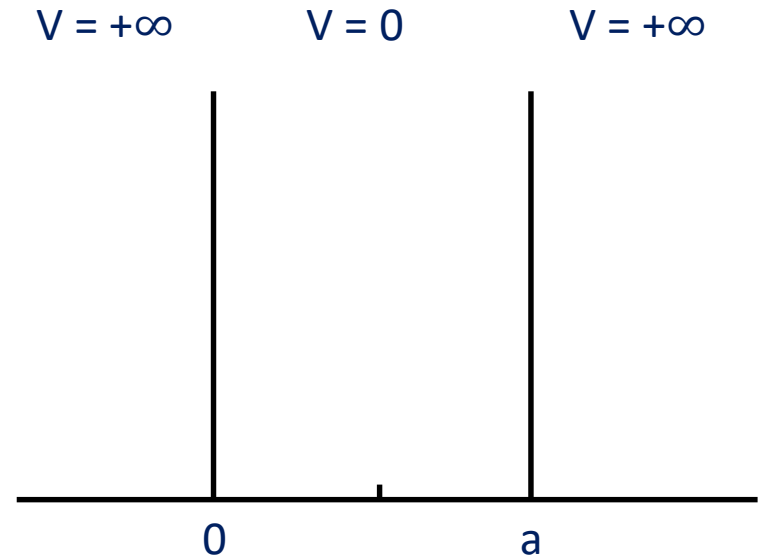
Conditions:

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

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

*for  $0 < x < a$*

$$V(x) = 0$$



## 2.4 Electrons in Infinite Quantum Well

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

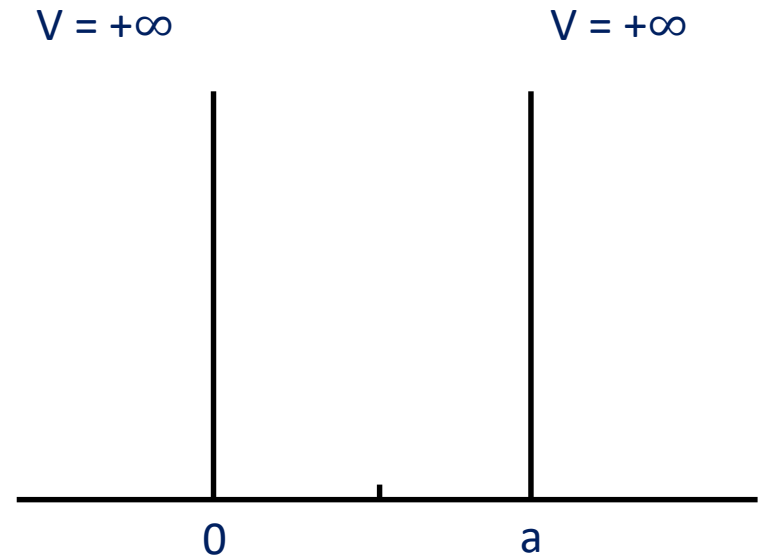
Conditions:

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

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

for  $0 < x < a$

$$V(x) = 0$$



$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$



$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{2mE}{\hbar^2} \Psi$$



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

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$



## 2.4 Electrons in Infinite Quantum Well

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$



$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{2mE}{\hbar^2} \Psi$$



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

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

The general solution

$$\Psi(x) = Ae^{-ikx} + Be^{ikx}$$

Boundary conditions:

$$\begin{cases} \Psi(x)|_{x=a,0} = 0 \\ \int_0^a \Psi(x)\Psi^*(x)dx = 1 \end{cases}$$

## 2.4 Electrons in Infinite Quantum Well

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The general solution

$$\Psi(x) = Ae^{-ikx} + Be^{ikx}$$

Boundary conditions:

$$\begin{cases} \Psi(x)|_{x=0} = 0 \\ \int_0^a \Psi(x)\Psi^*(x)dx = 1 \end{cases}$$

$$\Psi(x) = Ae^{-ik0} + Be^{ik0} = 0 \Rightarrow A = -B$$

$$\Psi(x) = Ae^{-ika} + Be^{ika} = 0 \Rightarrow \sin(ka) = 0$$

$$ka = n\pi \quad \text{where } n = 0, \pm 1, \pm 2, \dots$$

## 2.4 Electrons in Infinite Quantum Well

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$



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$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

The general solution

$$\Psi(x) = Ae^{-ikx} + Be^{ikx}$$

Boundary conditions:

$$\begin{cases} \Psi(x)|_{x=a,0} = 0 \\ \int_0^a \Psi(x)\Psi^*(x)dx = 1 \end{cases} \Rightarrow \begin{aligned} k &= \frac{n\pi}{a} \quad n = 0, \pm 1, \pm 2, \dots \\ E &= \frac{k^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \end{aligned}$$

## 2.4 Electrons in Infinite Quantum Well

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

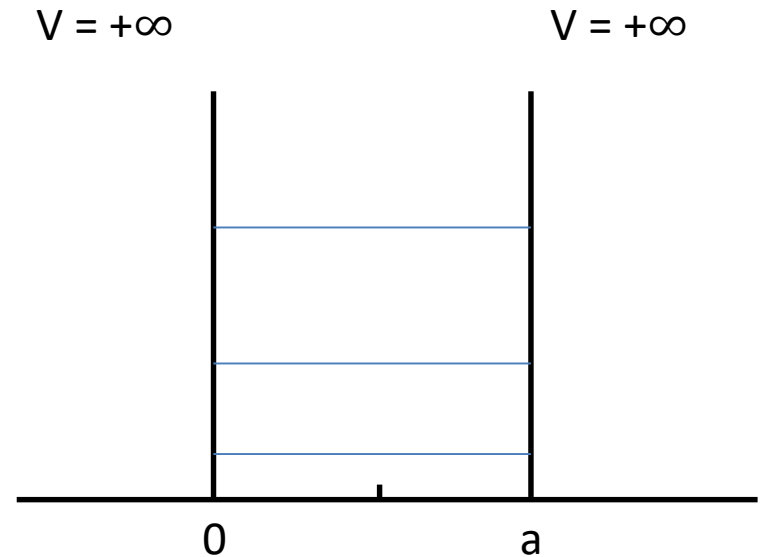
Conditions:

$$\text{for } x \leq 0, x \geq a$$

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

$$\text{for } 0 < x < a$$

$$V(x) = 0$$

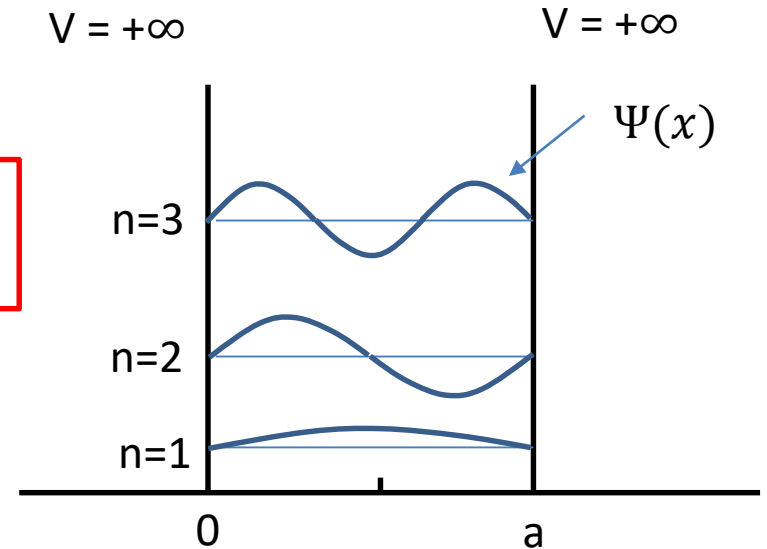
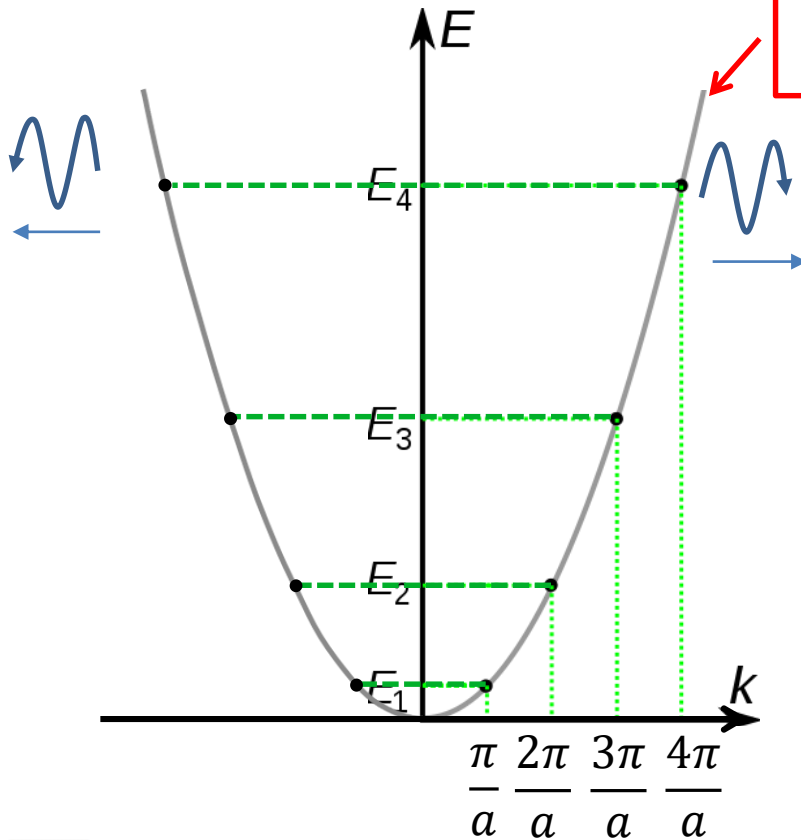


$$E = \frac{k^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

## 2.4 Electrons in Infinite Quantum Well

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

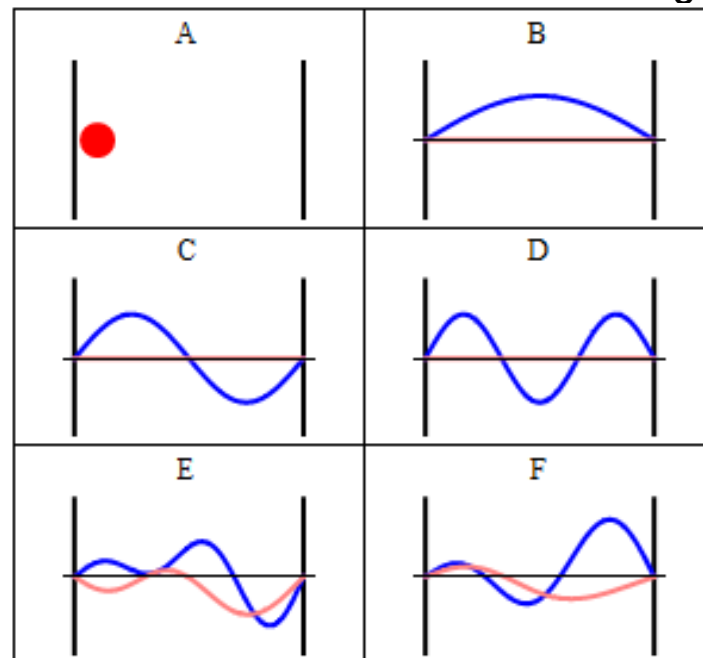
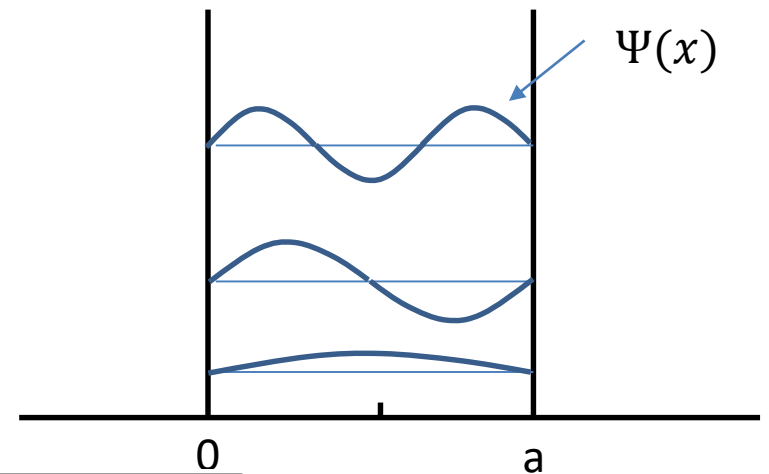
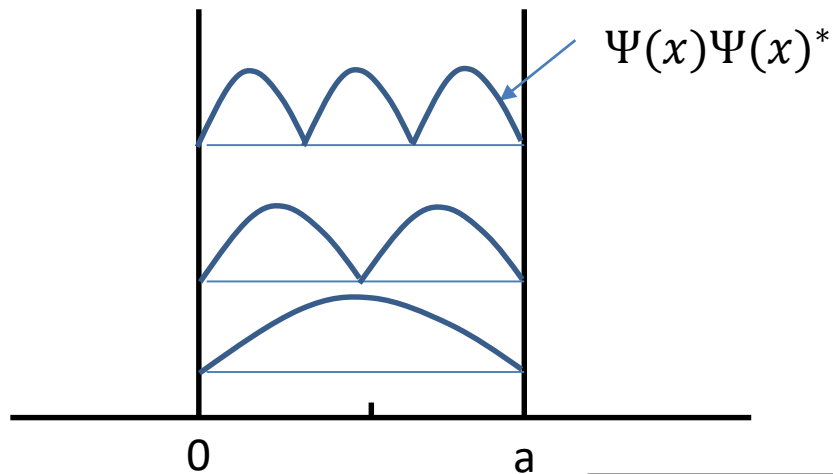
$$E = \frac{k^2 \hbar^2}{2m}$$



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

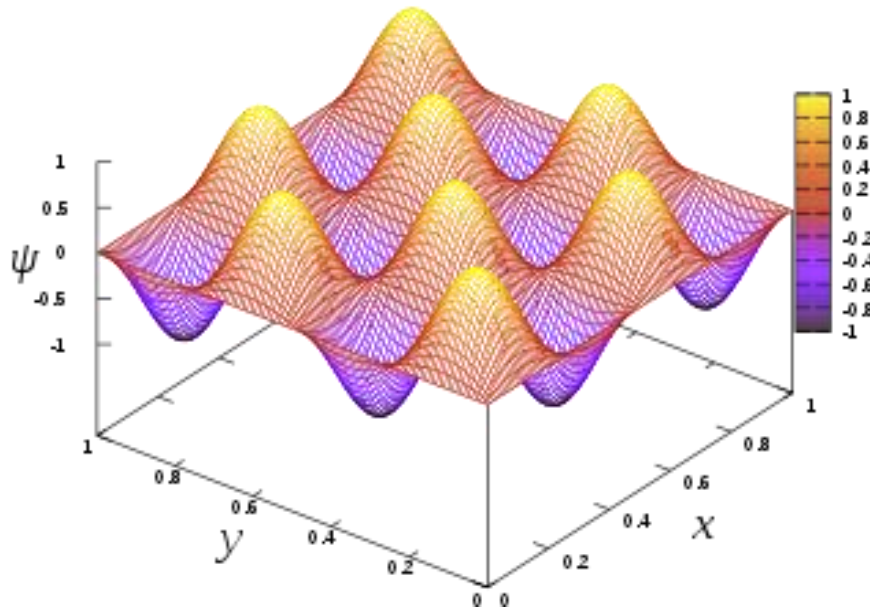
$$k = \frac{n\pi}{a} \quad n = 0, \pm 1, \pm 2, \dots$$

## 2.4 Electrons in Infinite Quantum Well

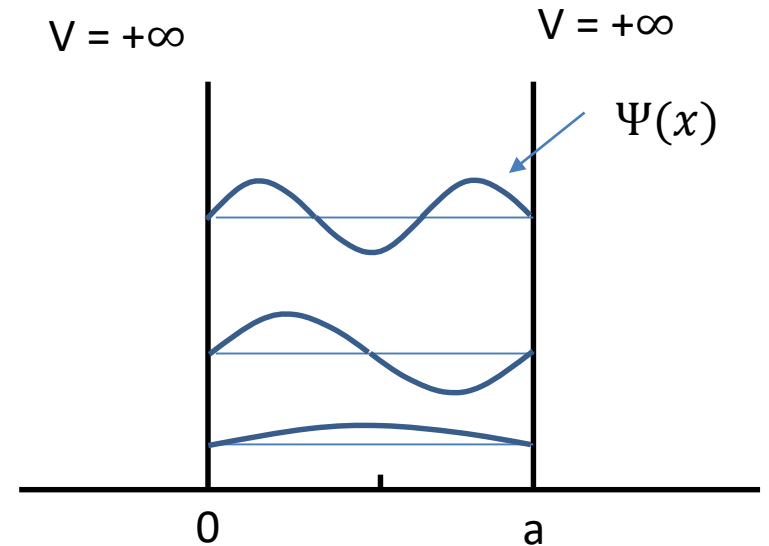


## 2.4 Electrons in Infinite Quantum Well

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



2-dimentional Quantum well



[http://en.wikipedia.org/wiki/Particle\\_in\\_a\\_box](http://en.wikipedia.org/wiki/Particle_in_a_box)

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

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2.6 Electrons in an atom



## 2.5 Electrons in Finite Quantum Well

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

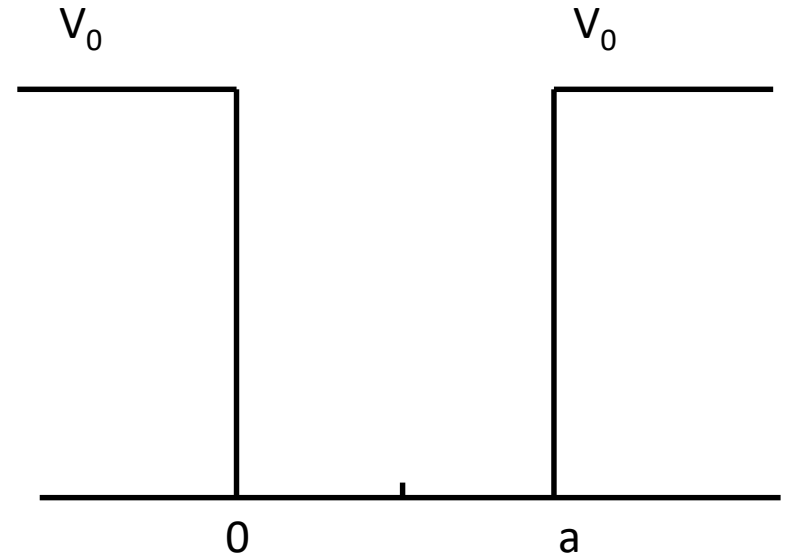
Conditions:

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

$$V(x) = V_0;$$

*for  $0 < x < a$*

$$V(x) = 0$$



## 2.5 Electrons in Finite Quantum Well

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

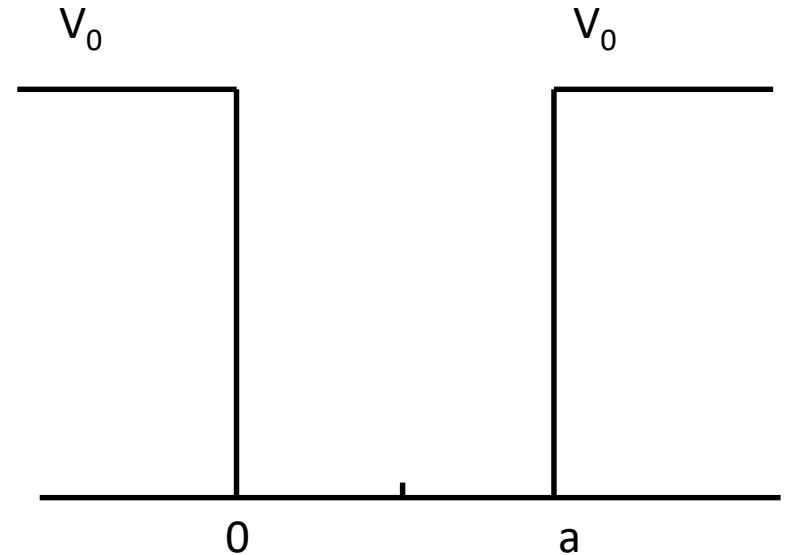
Conditions:

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

$$V(x) = V_0;$$

for  $0 < x < a$

$$V(x) = 0$$



$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = (E - V_0)\Psi$$

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

$$k_1 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$

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

$$k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$

## 2.5 Electrons in Finite Quantum Well

Boundary Conditions:

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

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

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

for  $x < 0, x > a$

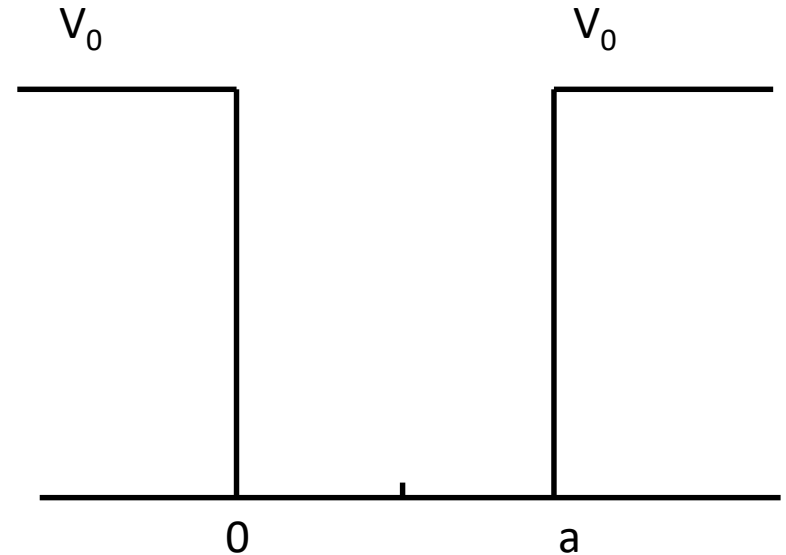
$$\Psi(x) = Ae^{-ik_1x} + Be^{ik_1x}$$

$$k_1 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

for  $0 \leq x \leq a$

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

$$k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$



## 2.5 Electrons in Finite Quantum Well

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

Boundary Conditions:

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

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

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

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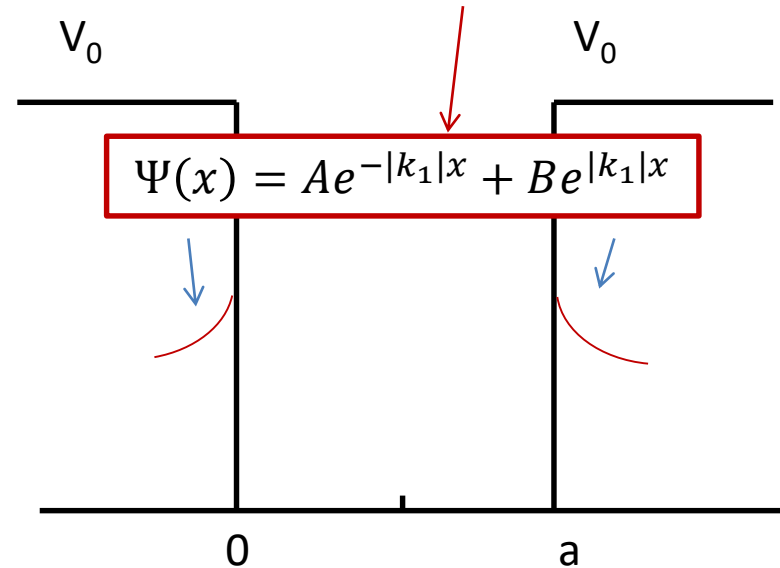
$$\Psi(x) = Ae^{-ik_1x} + Be^{ik_1x}$$

$$k_1 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

for  $0 \leq x \leq a$

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

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## 2.5 Electrons in Finite Quantum Well

Boundary Conditions:

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

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

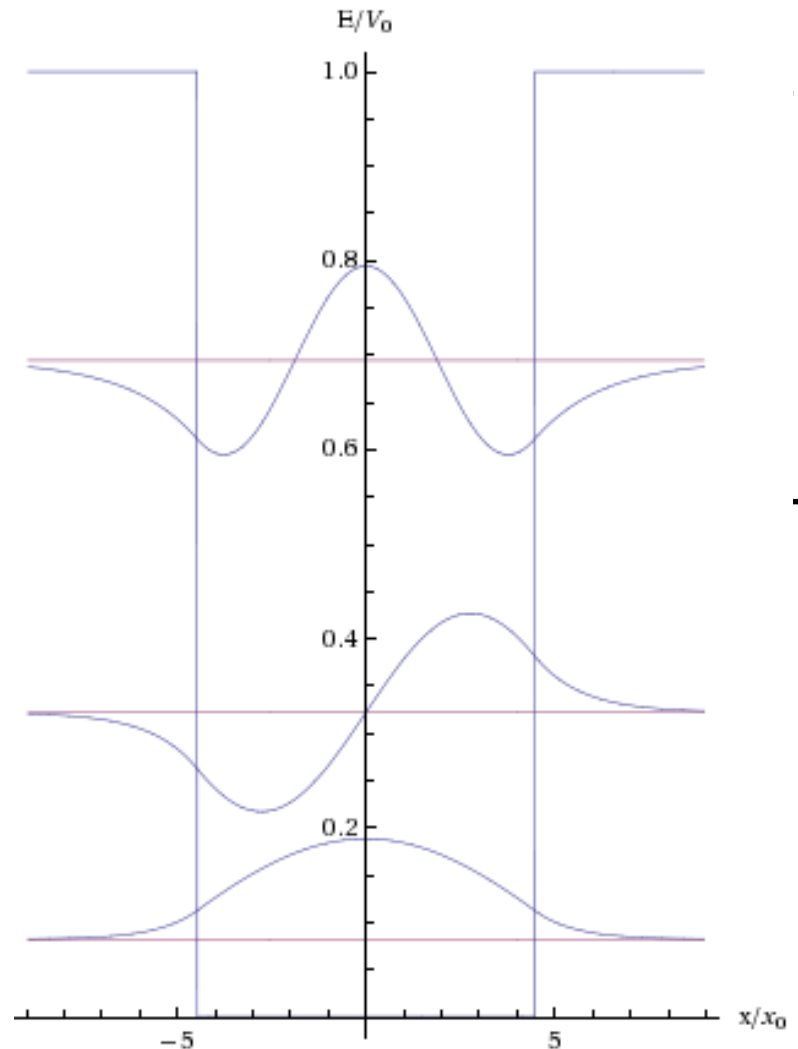
$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1$$

for  $x < 0, x > a$

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

for  $0 \leq x \leq a$

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



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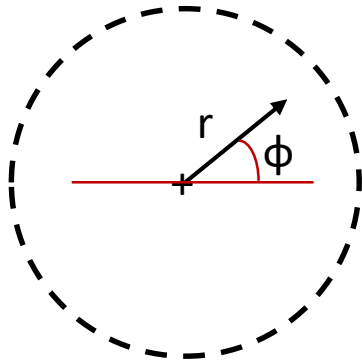
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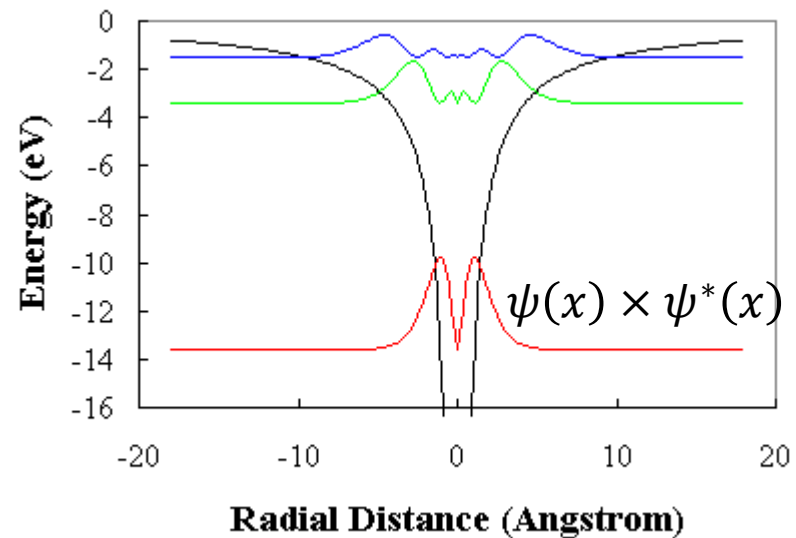
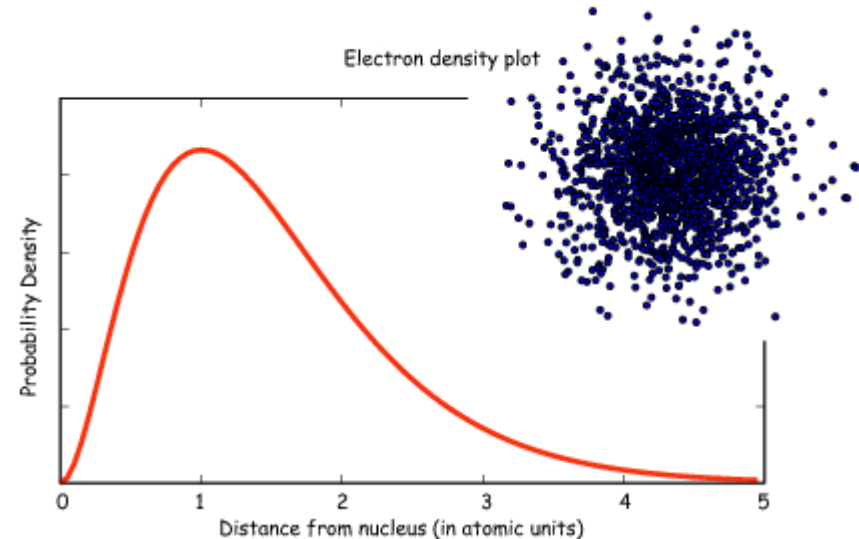
**2.6 Electrons in an atom**

## 2.6 Electrons in an Atom

- 2D

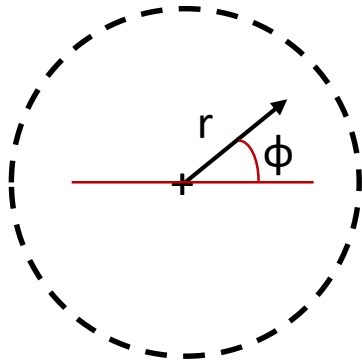


Periodic boundary conditions

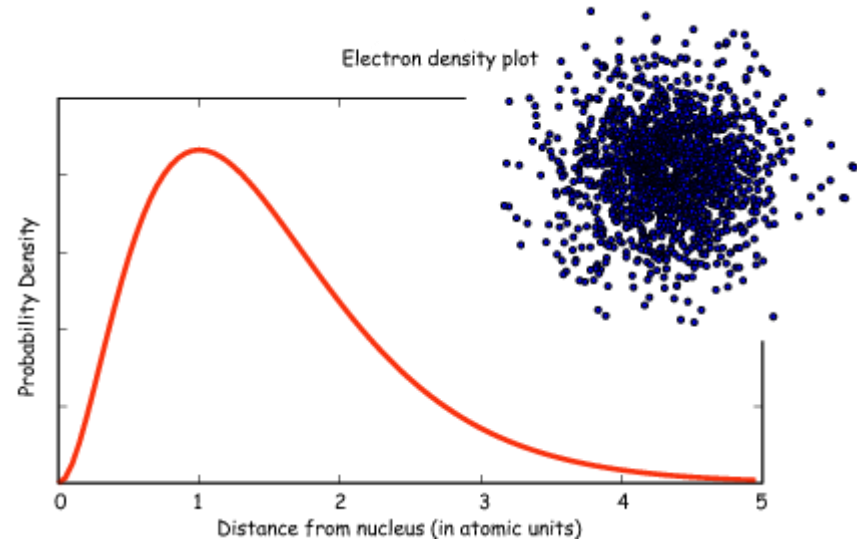


## 2.6 Electrons in an Atom

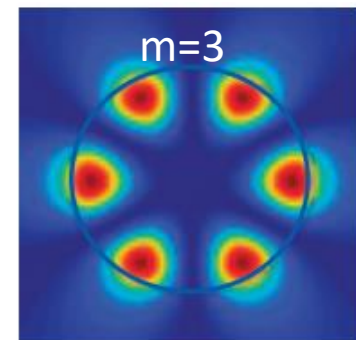
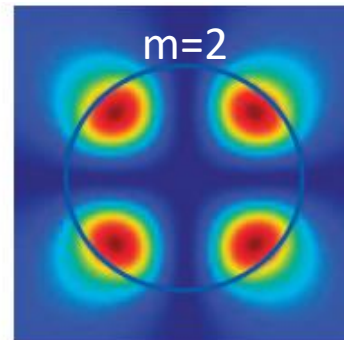
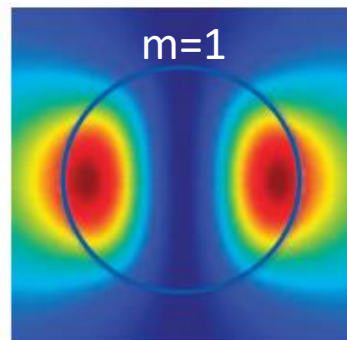
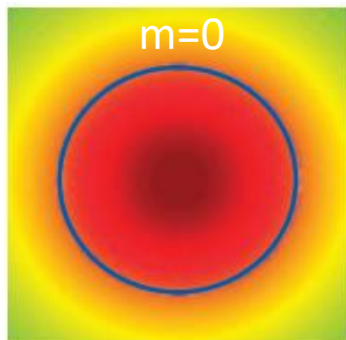
- 2D



Periodic boundary conditions



$f(r, \phi)$

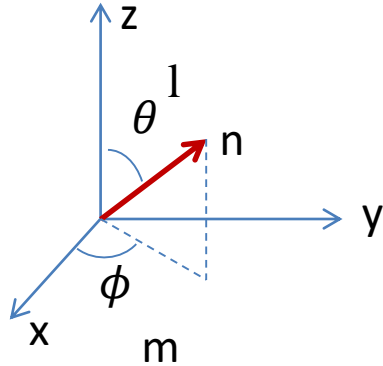




## 2.6 Electrons in an Atom

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- 3D



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

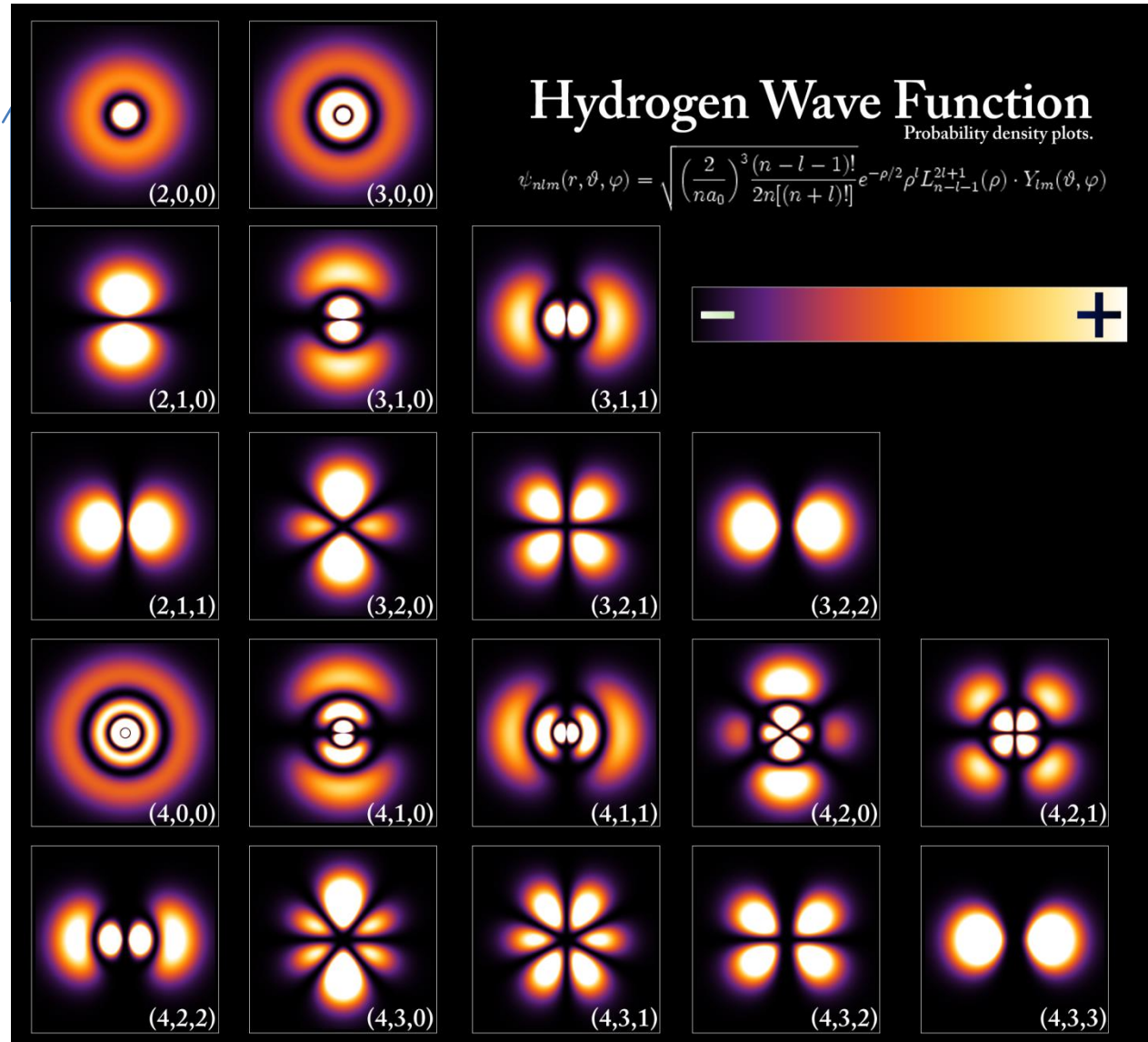
## 2.6 Electrons in an Atom

- 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 (shape: s,p)

Element	Notation	$n(\text{orbital})$	$l$	$m$	$s$
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	<div style="display: flex; align-items: center; justify-content: center;"> <div style="margin-right: 10px;"> <math>m=0, -1, 1</math> </div> <div style="border: 1px solid black; padding: 5px; text-align: center;"> <div style="display: flex; justify-content: space-around;"> <div style="border: 1px solid black; padding: 2px;"><math>\uparrow\downarrow</math></div> <div style="border: 1px solid black; padding: 2px;"><math>\uparrow\downarrow</math></div> <div style="border: 1px solid black; padding: 2px;"><math>\uparrow</math></div> <div style="border: 1px solid black; padding: 2px; width: 20px;"></div> <div style="border: 1px solid black; padding: 2px; width: 20px;"></div> </div> </div> </div>	$m = 0, -1, +1$ $s = +\frac{1}{2}, -\frac{1}{2}$
Carbon	$1s^2 2s^2 2p^2$	2	1		
Nitrogen	$1s^2 2s^2 2p^3$	2	1		
Oxygen	$1s^2 2s^2 2p^4$	2	1		
Fluorine	$1s^2 2s^2 2p^5$	2	1		
Neon	$1s^2 2s^2 2p^6$	2	1		

$1s$

$n=1$

$l=0$

$2s$

$n=2$

$l=0$

$2p$

$n=2$

$l=1$