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 2nd 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 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: $b^2 Ae^{bx} = k^2 Ae^{bx}$

$$\Rightarrow b = \pm k$$

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

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

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 2nd order differential equations and waves

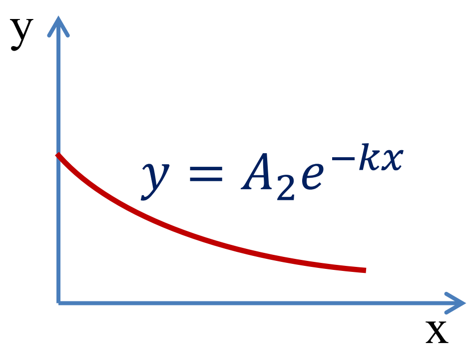
$$\frac{\partial^2 y}{\partial x^2} = k^2 y$$

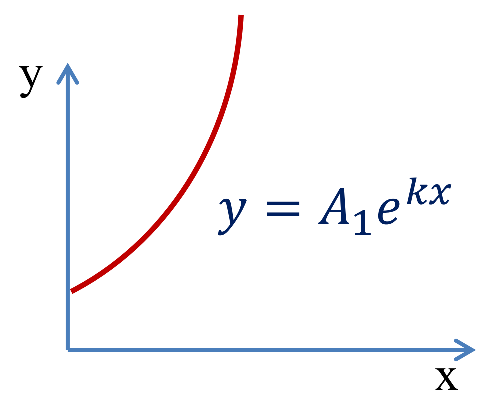
General solution: $y = Ae^{bx}$

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

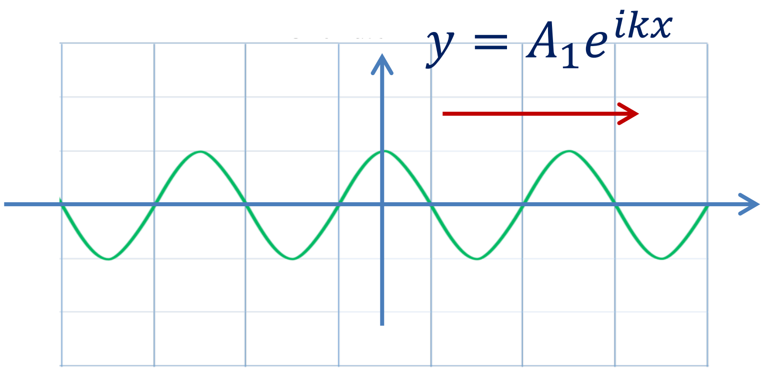
$$\Rightarrow b = \pm k$$

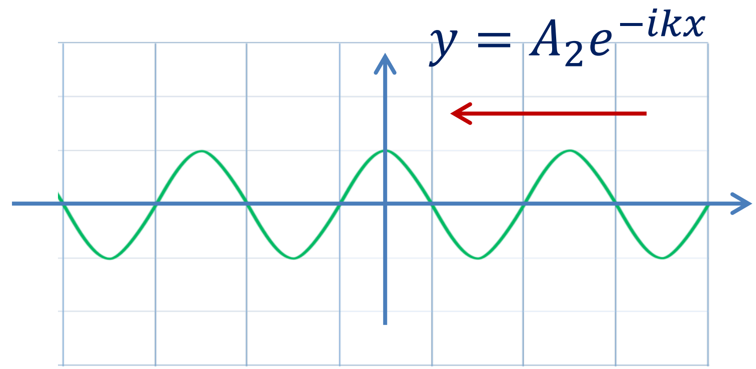
$$\Rightarrow y = A_1 e^{kx} + A_2 e^{-kx}$$





2.1 2nd order differential equations and waves





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

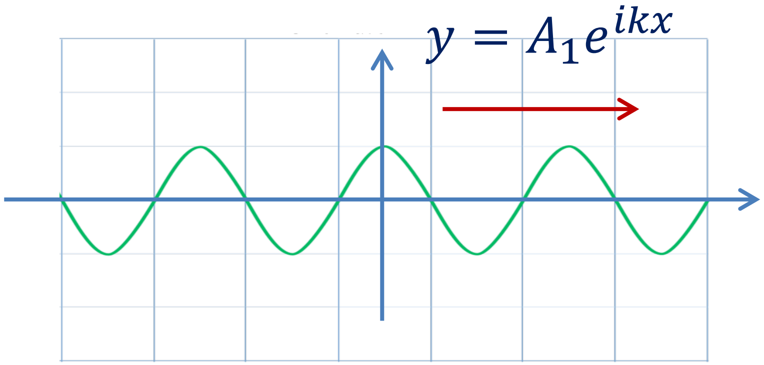
General solution: $y = Ae^{bx}$

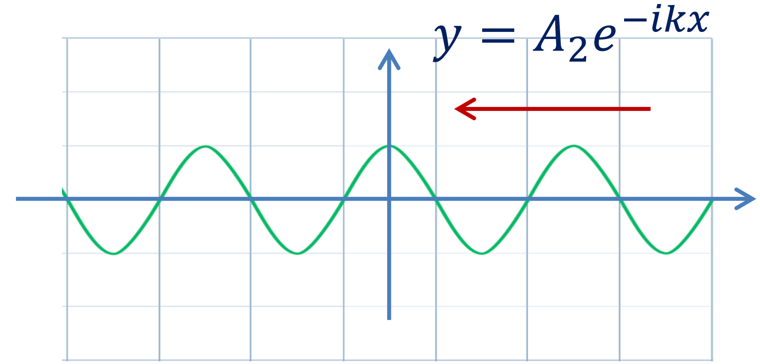
Plug into the equation: $b^2 A e^{bx} = -k^2 A e^{bx}$

$$\Rightarrow b = \pm ki$$

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

2.1 2nd order differential equations and waves



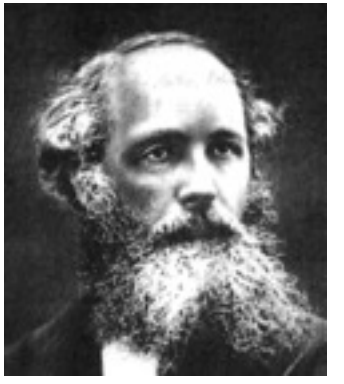


1. Give a wave propagating along x with a wavelength λ_0, please write the static 2nd order differential equation that governs the behavior of this wave.

2.1 2nd order differential equations and waves

- Electromagnetic (EM) wave

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



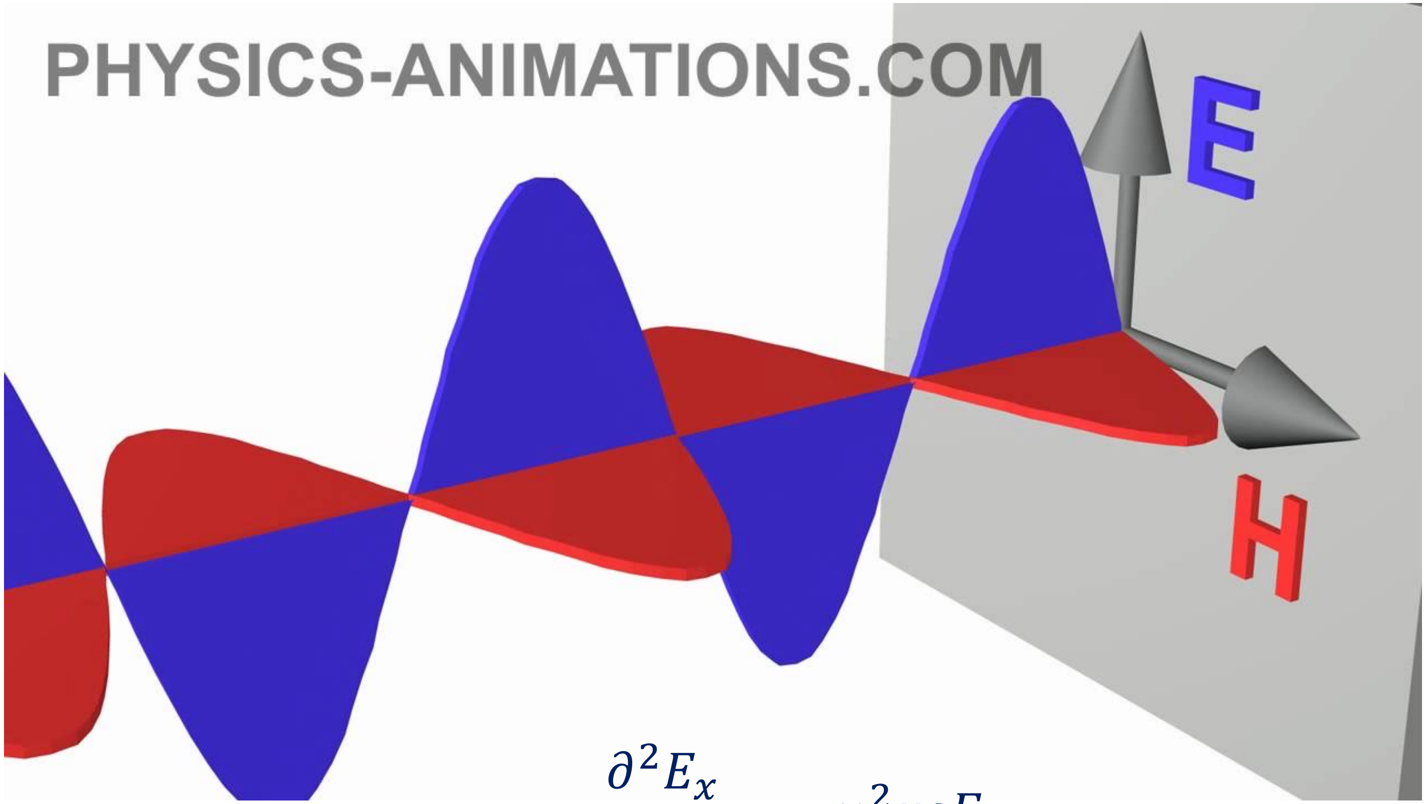
James Maxwell

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

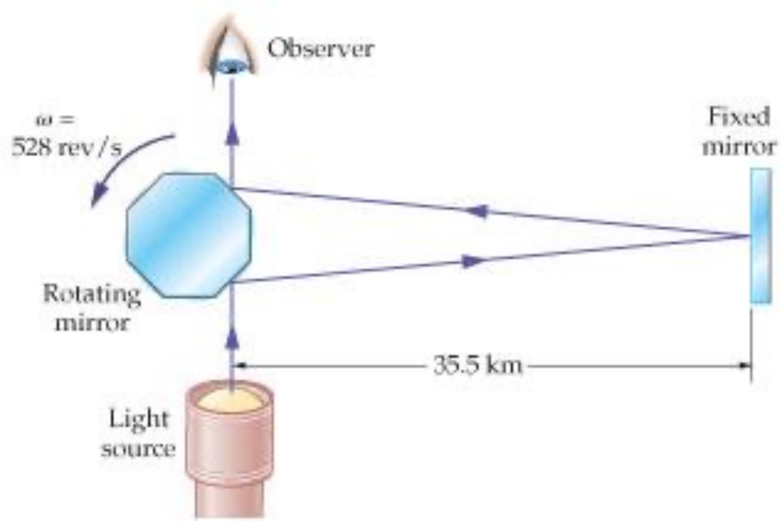
2.4 Electrons in infinite quantum well

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



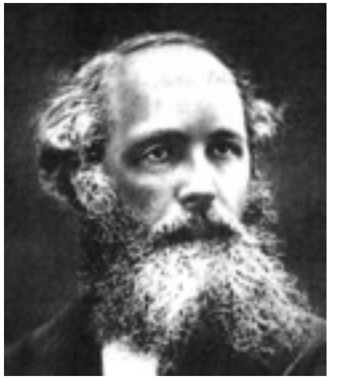
Rotation mirror

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

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

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

$\boxed{\text{Light is an electromagnetic wave!}}$

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

2.2 Historic events in developing quantum mechanics

③ Light wave-particle duality in 1905

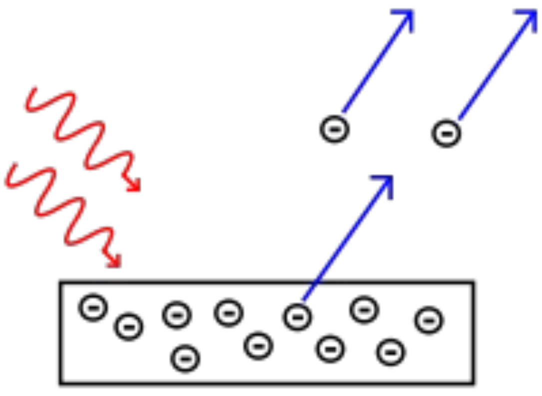
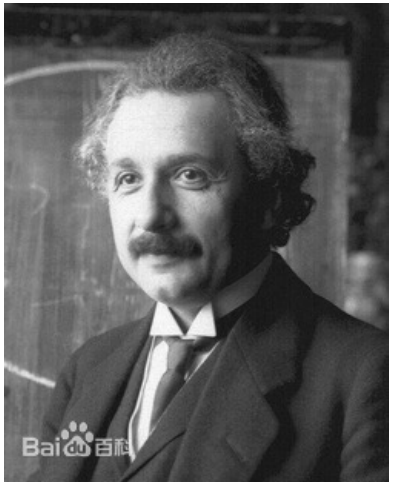


Photo-electric experiment

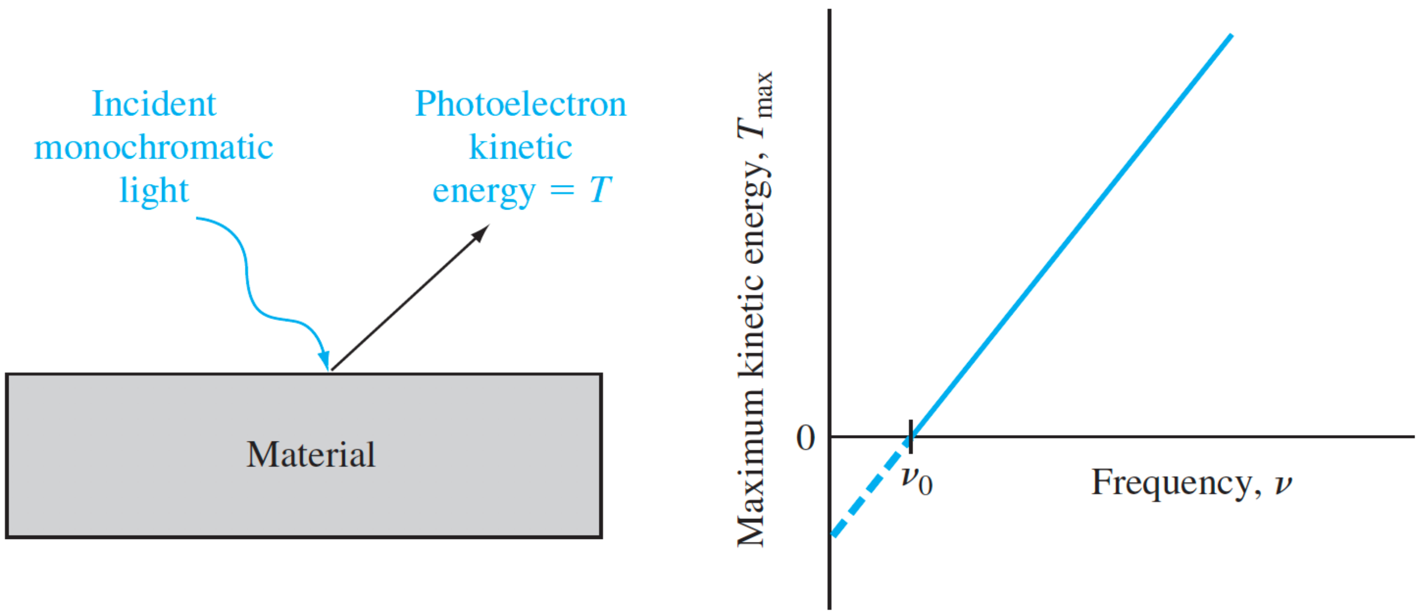


Albert Einstein
Nobel Prize 1921

- 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



(a) (b)

- 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

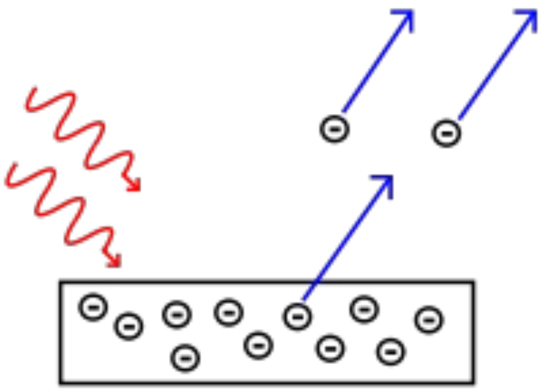
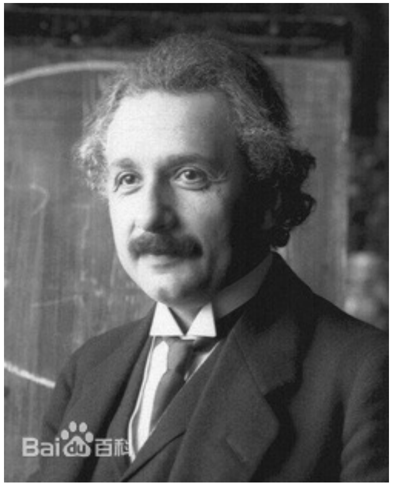


Photo-electric experiment



Albert Einstein
Nobel Prize 1921

$$E = h\text{v} = \hbar\omega \qquad\qquad E = mc^2$$

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

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

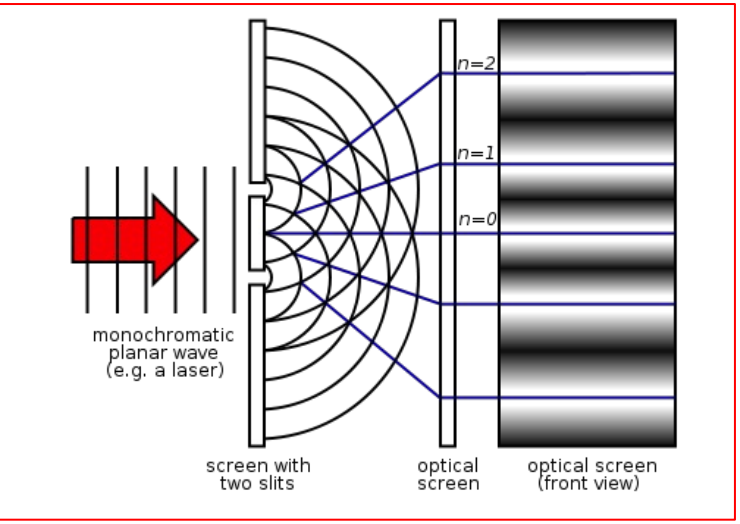
$$E = \frac{1}{2}mv^2 \qquad E = h\text{v} = \hbar\omega$$

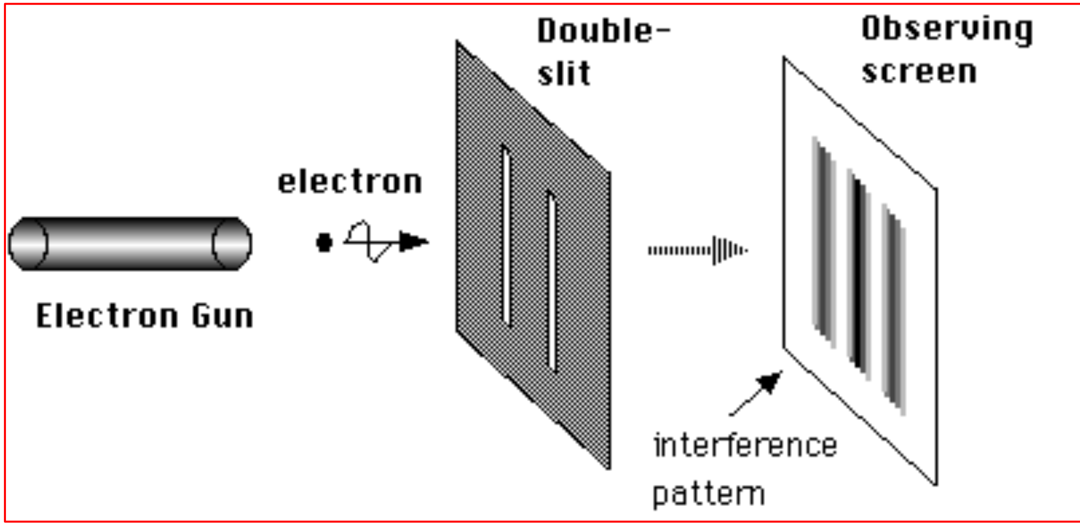
$$\text{p} = mv \qquad \text{p} = \frac{h}{\lambda} = \hbar k$$

Matter particle Wave- particle

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

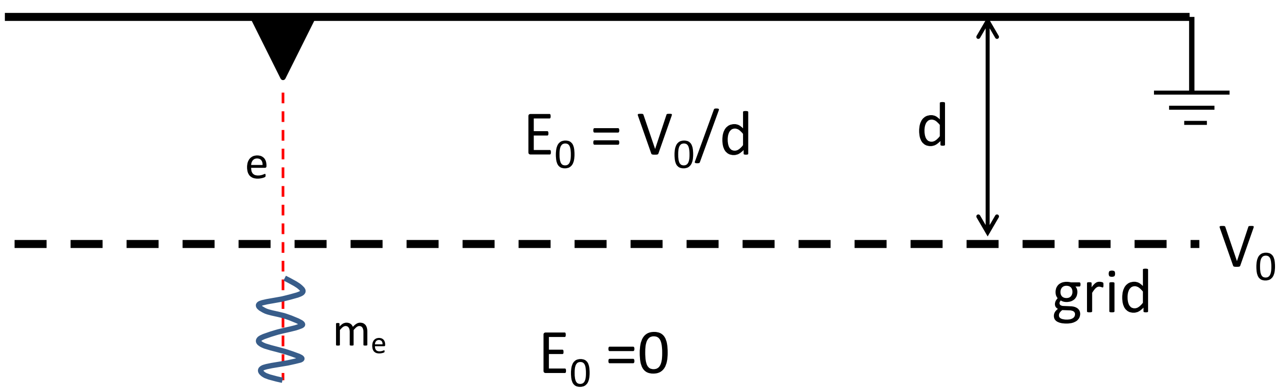
$$\frac{\partial^2 y}{\partial x^2} = -k^2 y$$

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

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

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

Quiz #1:



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

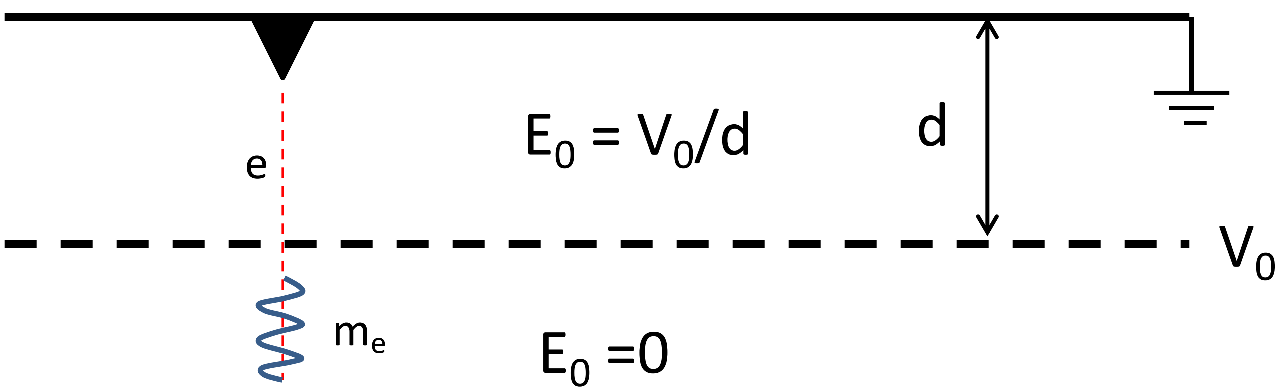
2.3 A case study

$$E = qV_0 = \frac{1}{2}mv^2 \qquad E = h\nu = \hbar\omega \qquad v = \sqrt{\frac{2qV_0}{m}}$$

$$\mathrm{p} = mv \qquad \mathrm{p} = \frac{h}{\lambda} = \hbar k \qquad k = \frac{m}{\hbar}v = \sqrt{\frac{2mqV_0}{\hbar^2}}$$

$$\frac{\partial^2\Psi}{\partial x^2} = -k^2\Psi = -\frac{2mqV_0}{\hbar^2}\Psi \qquad \boxed{\Rightarrow \;\; -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = E\Psi} \qquad \boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi = E\Psi}$$

Schrodinger Equation !



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

Outline

2.1 2nd 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

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

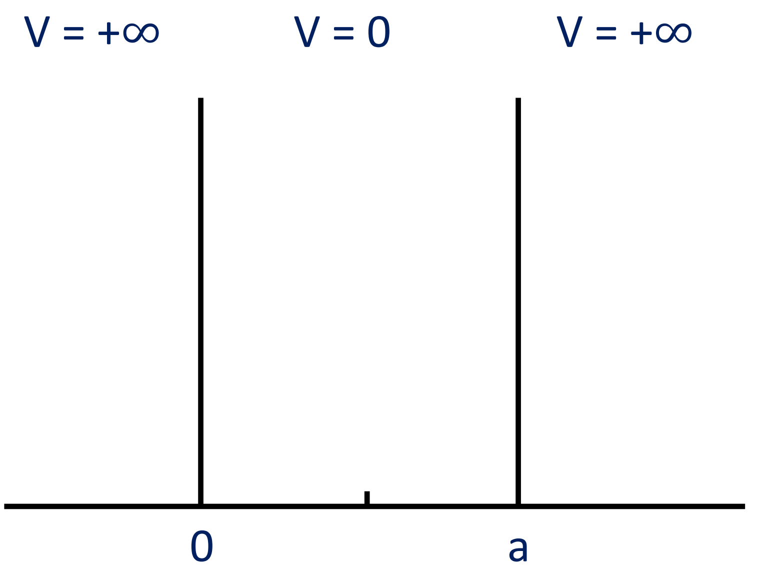
Conditions:

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

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

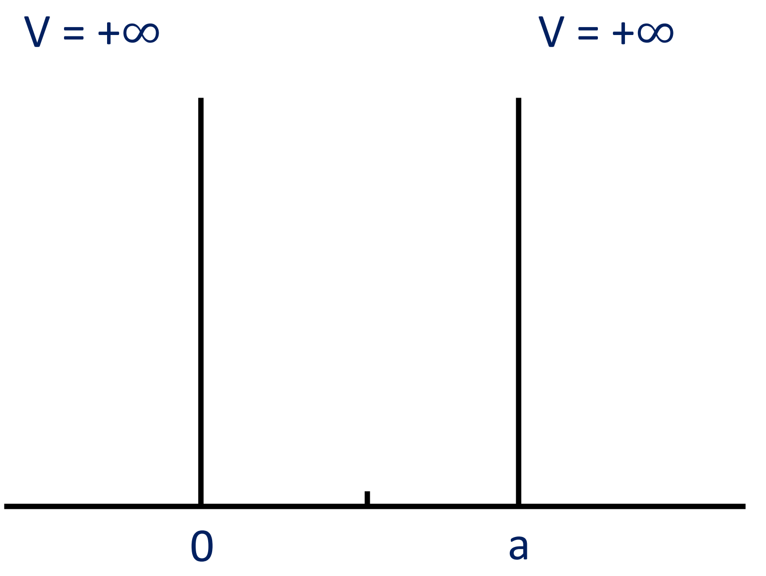
$$for\ 0 < x < a$$

$$V(x) = 0$$



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:

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

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

$for\ 0 < x < a$

$$V(x) = 0$$

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

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

2.4 Electrons in Infinite Quantum Well

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

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

The general solution

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

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

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

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

The general solution

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

Boundary conditions:

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

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

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

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

2.4 Electrons in Infinite Quantum Well

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

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

The general solution

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

Boundary conditions:

$$\begin{cases} \Psi(x)|_{x=a,0} = 0 \\ \int_0^a \Psi(x)\Psi^*(x)dx = 1 \end{cases} \Rightarrow k = \frac{n\pi}{a} \quad n = 0, \pm 1, \pm 2, \ldots$$

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

2.4 Electrons in Infinite Quantum Well

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

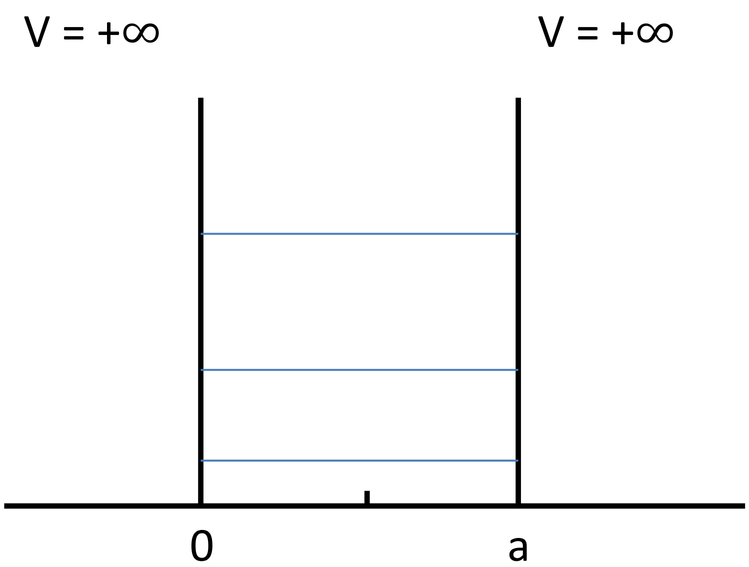
Conditions:

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

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

$for\ 0 < x < a$

$$V(x)=0$$

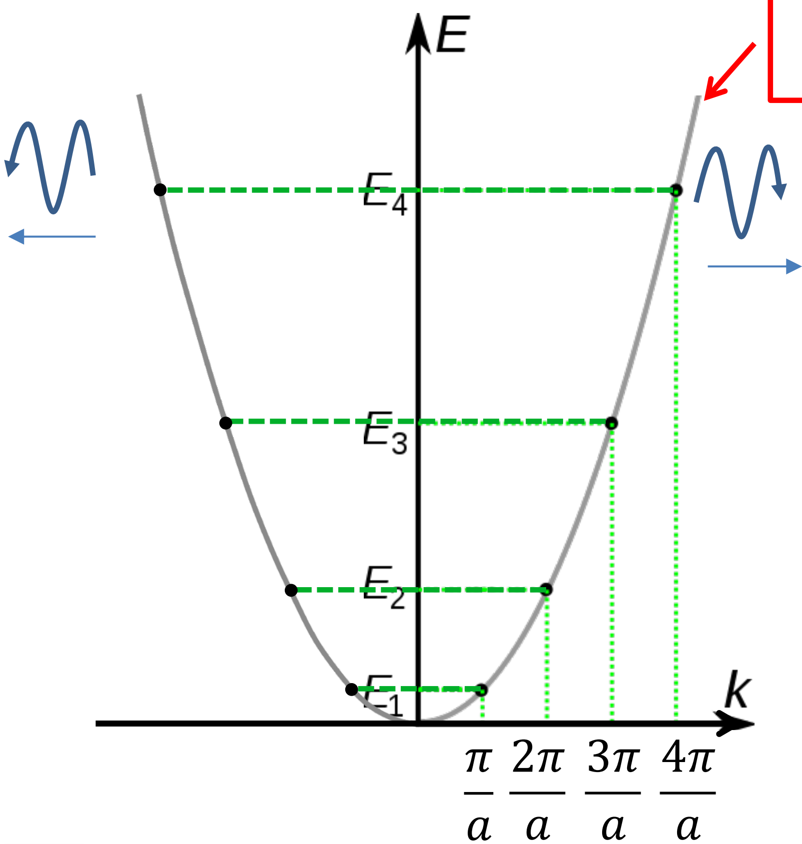


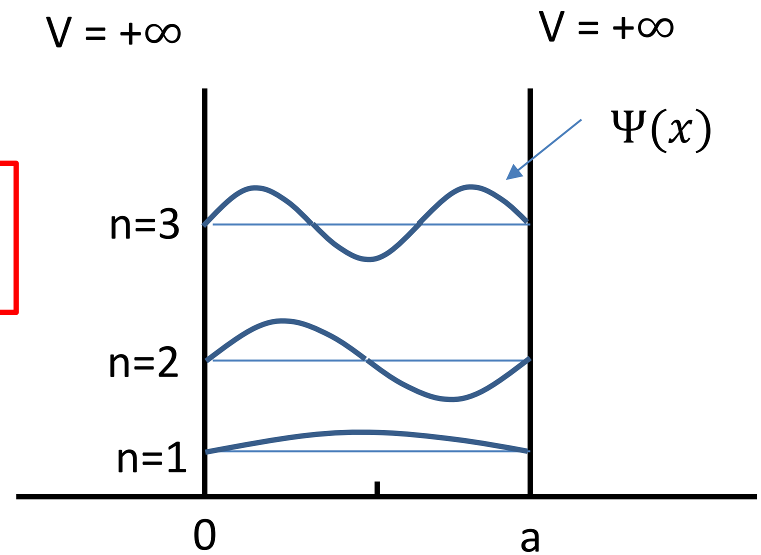
$$\mathrm{E}=\frac{k^2\hbar^2}{2m}=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

2.4 Electrons in Infinite Quantum Well

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

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

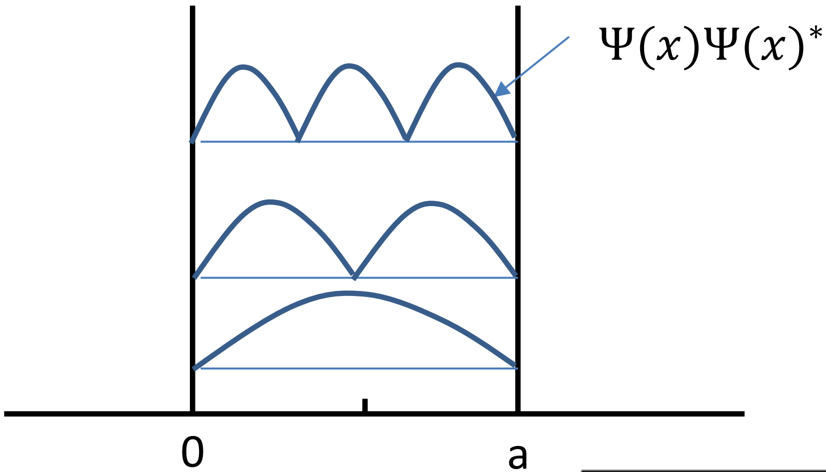


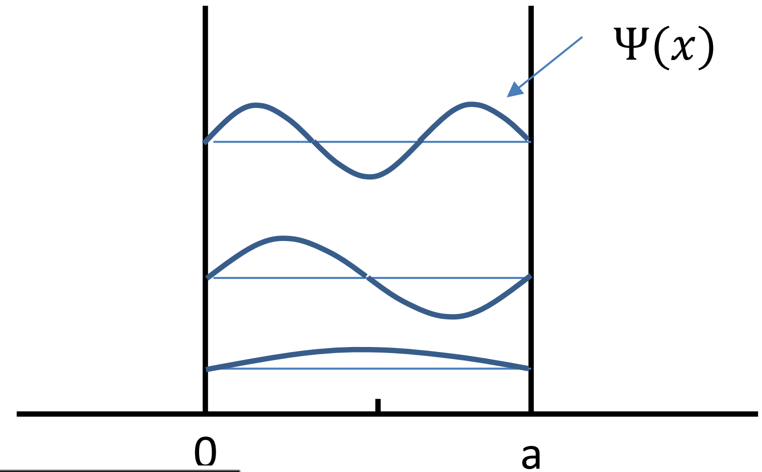


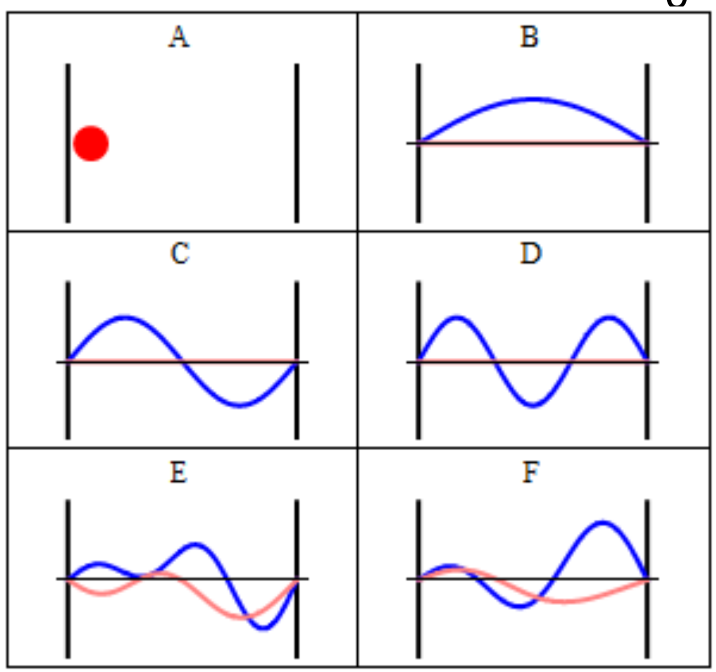
$$\mathrm{E}=\frac{k^2\hbar^2}{2m}=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

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

2.4 Electrons in Infinite Quantum Well

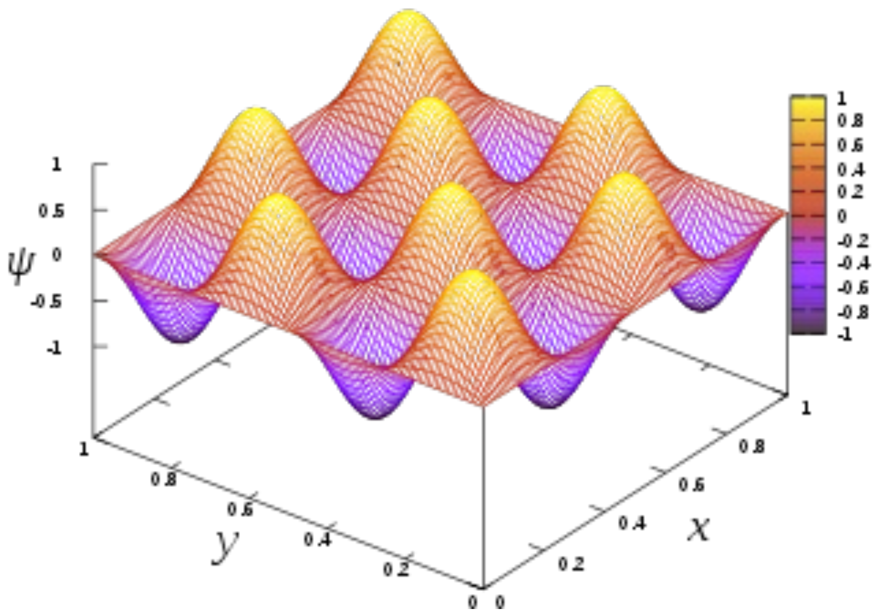




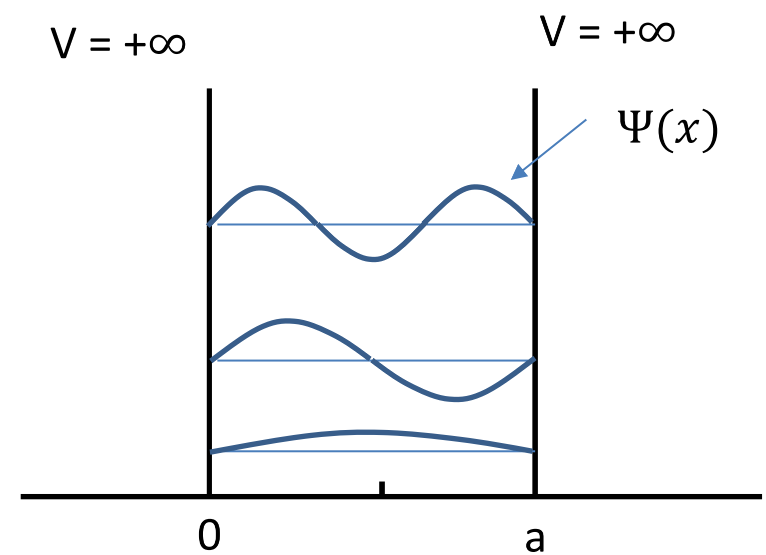


2.4 Electrons in Infinite Quantum Well

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



2-dimentional Quantum well



http://en.wikipedia.org/wiki/Particle_in_a_box

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

Outline

2.1 2nd order differential equations and waves

2.2 Historic events in developing quantum mechanics

2.3 A case study

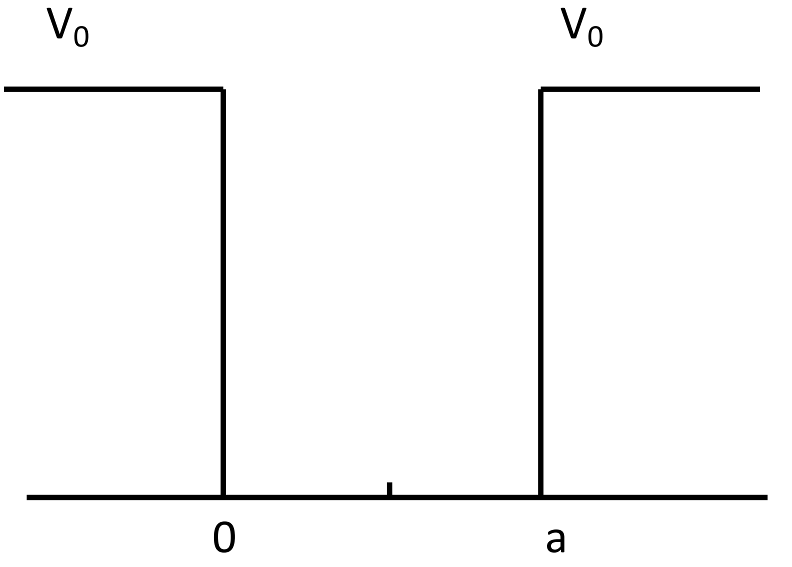
2.4 Electrons in infinite quantum well

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:

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

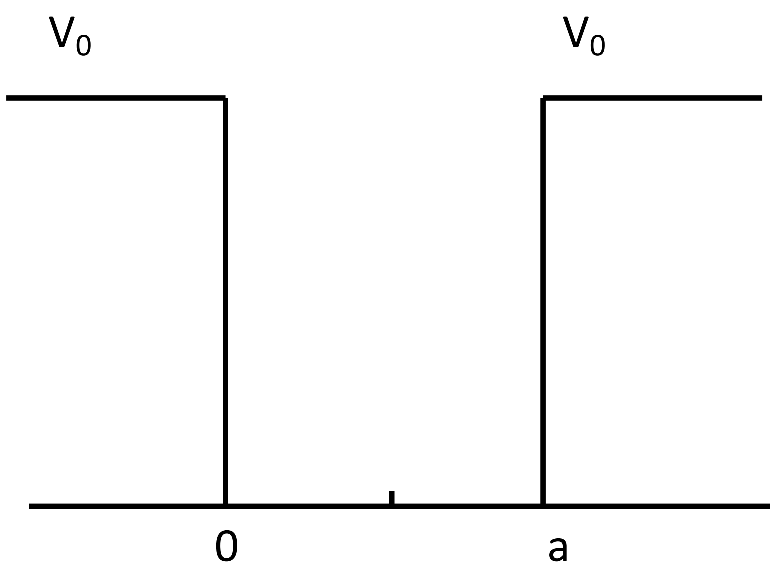
$$V(x) = V_0;$$

$for\ 0 < x < a$

$$V(x) = 0$$

2.5 Electrons in Finite Quantum Well

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



Conditions:

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

$$V(x) = V_0;$$

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

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

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

$for\ 0 < x < a$

$$V(x) = 0$$

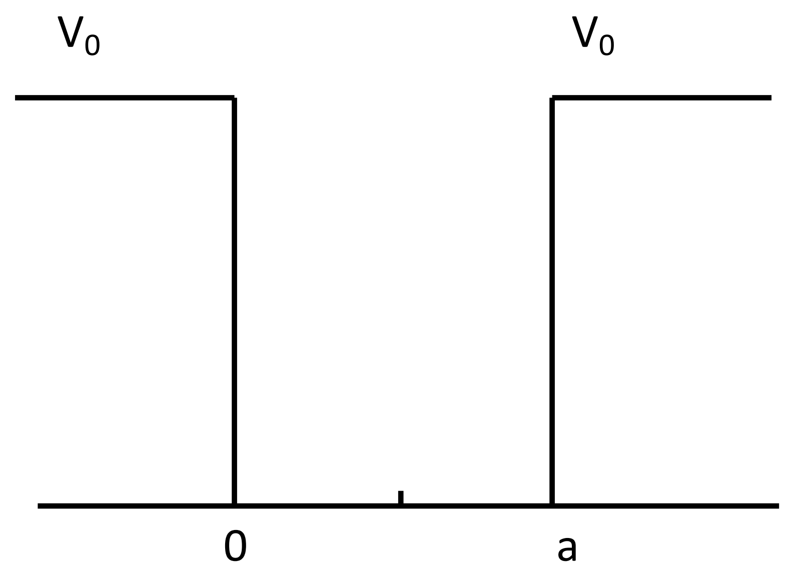
$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = E\Psi$$

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

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

2.5 Electrons in Finite Quantum Well

Boundary Conditions:



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

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

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

$for\ x < 0, x > a$

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

$for\ 0 \le x \le a$

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

2.5 Electrons in Finite Quantum Well

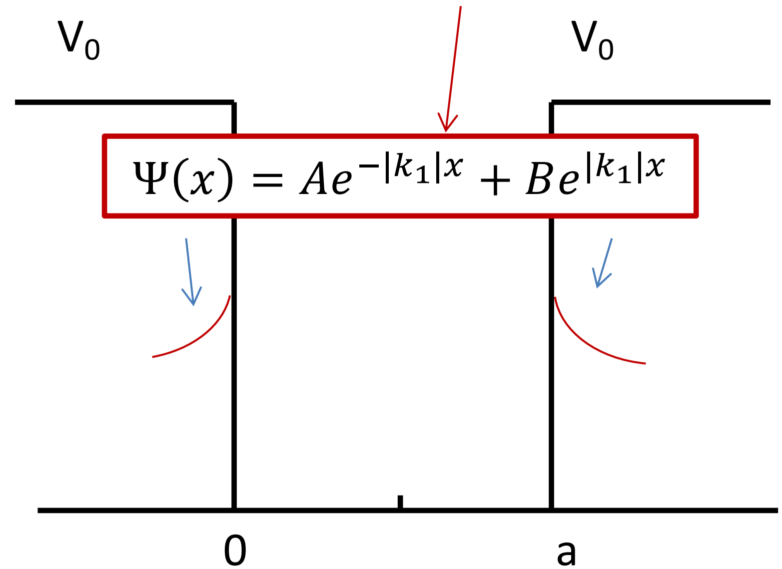
If E < V_0 $\quad k_1 = i\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$

Boundary Conditions:

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

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

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



$for\ x < 0, x > a$

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

$for\ 0 \le x \le a$

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

2.5 Electrons in Finite Quantum Well

Boundary Conditions:

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

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

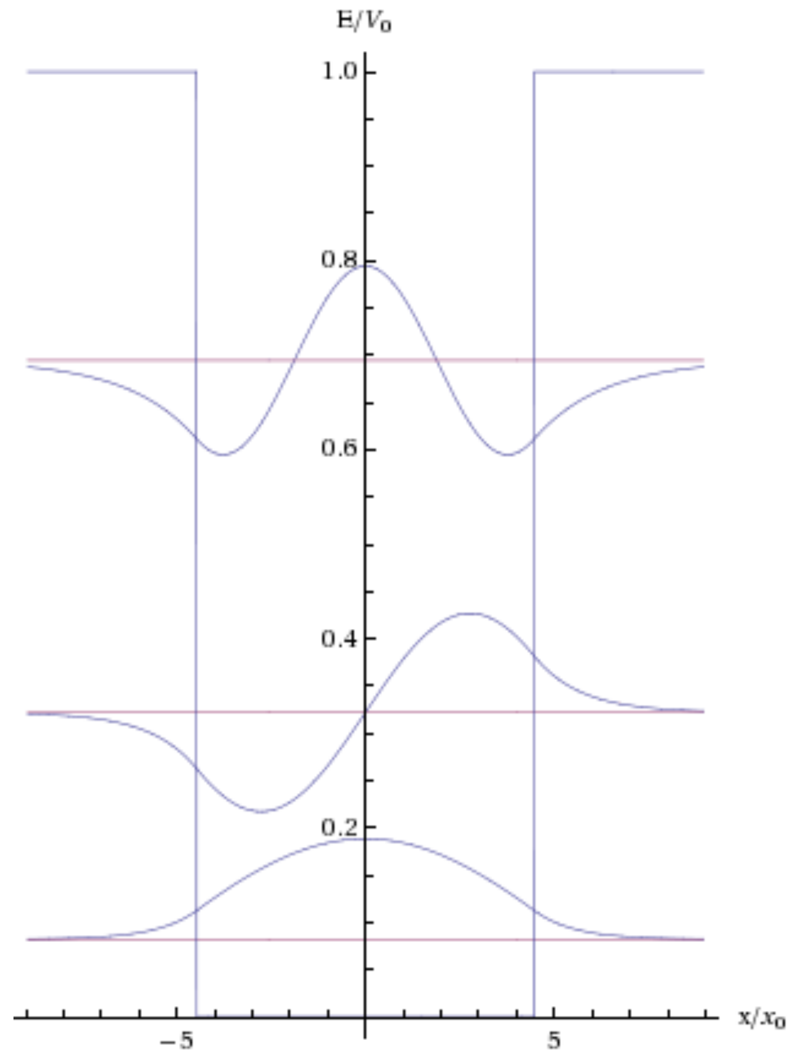
$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1$$

$for\ x < 0, x > a$

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

$for\ 0 \le x \le a$

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



Outline

2.1 2^{nd} order differential equations and waves

2.2 Historic events in developing quantum mechanics

2.3 A case study

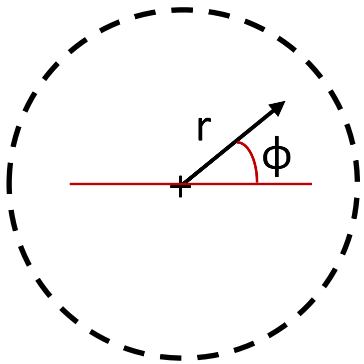
2.4 Electrons in infinite quantum well

2.5 Electrons in finite quantum well

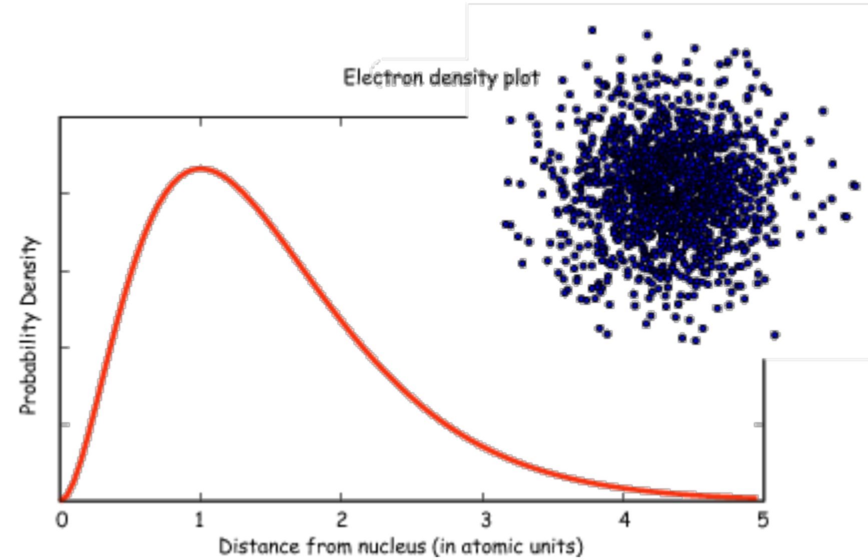
2.6 Electrons in an atom

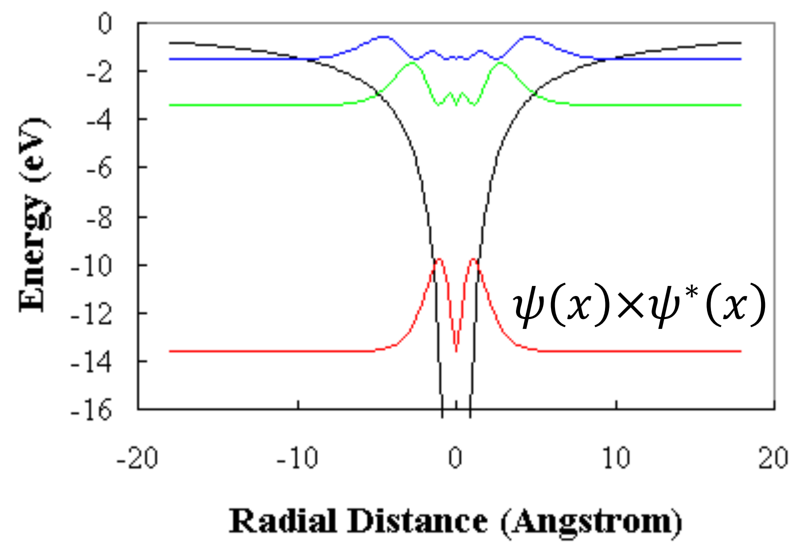
2.6 Electrons in an Atom

- 2D



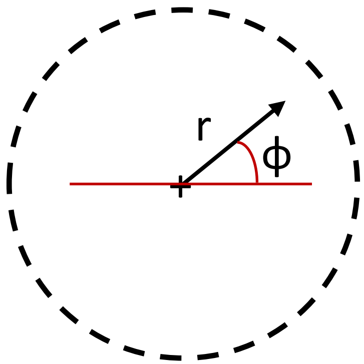
Periodic boundary conditions

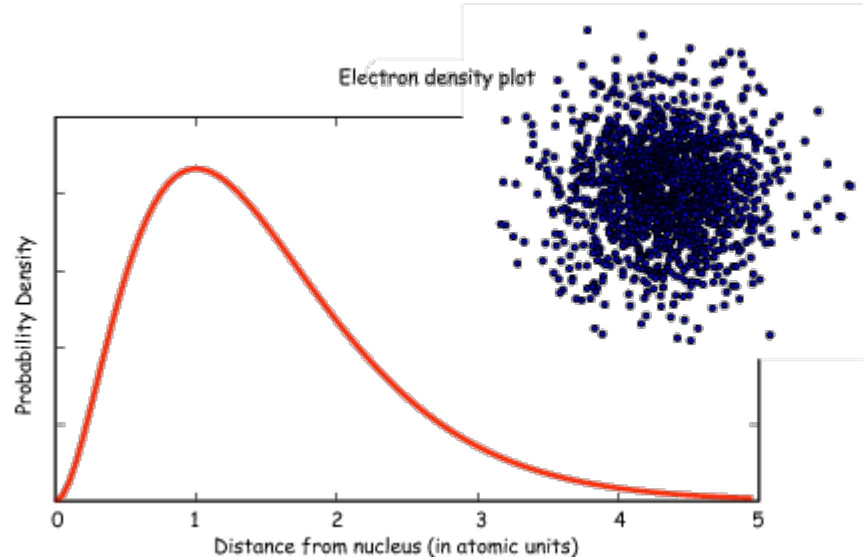




2.6 Electrons in an Atom

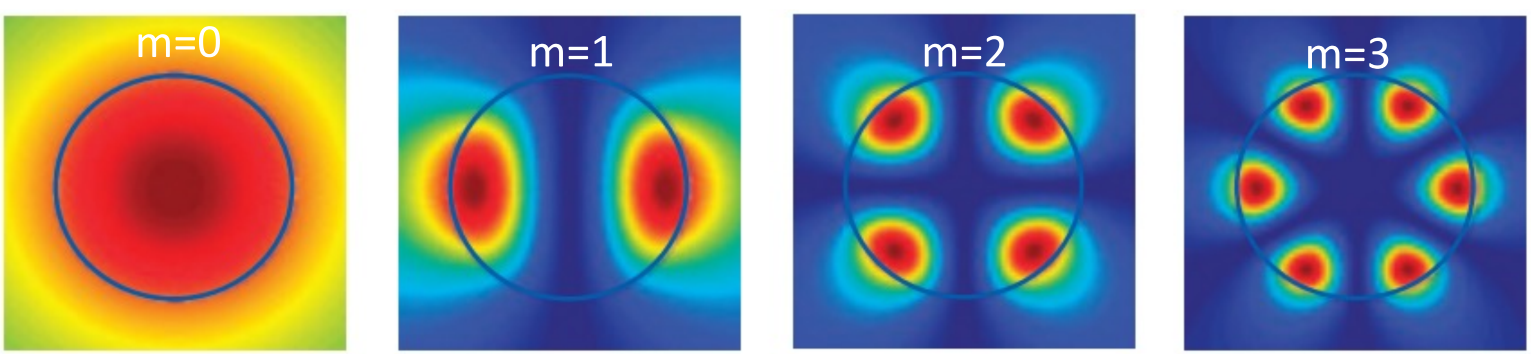
- <u>2D</u>





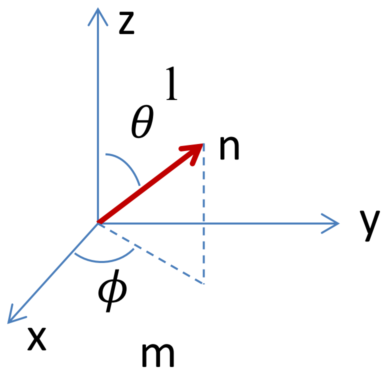
Periodic boundary conditions

$f(r, \phi)$



2.6 Electrons in an Atom

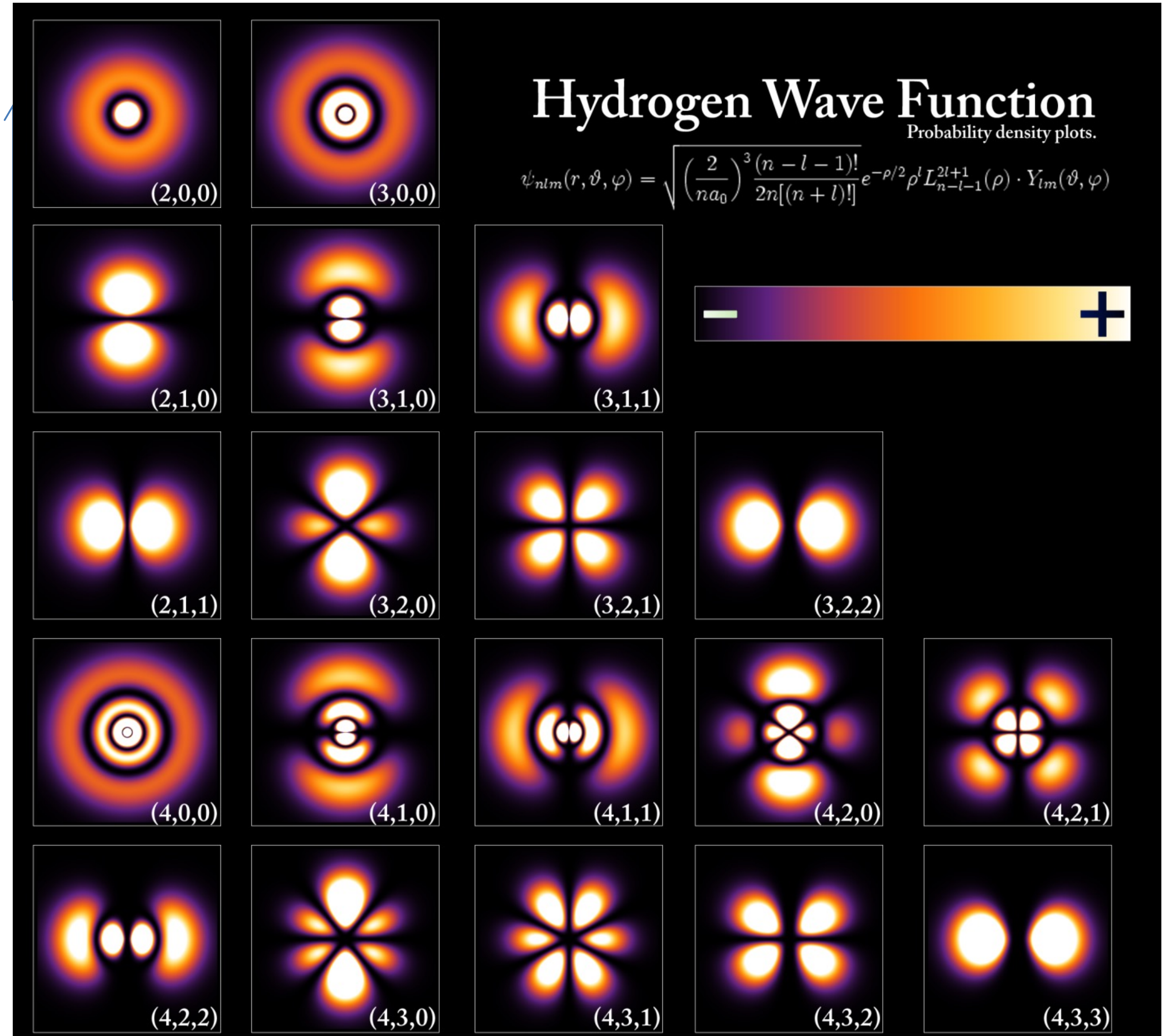
- 3D



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

2.6 Electrons in an Atom

- 3D



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

$2s^2 2p^6$

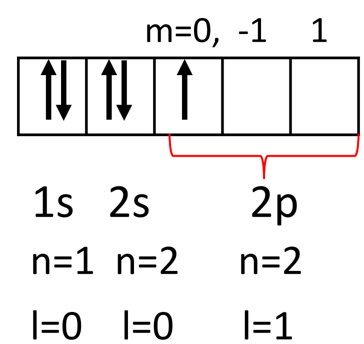
$1s^2$

2.6 Electrons in an Atom

- 3D

Table 2.1 | Initial portion of the periodic table (shape: s,p)

Element	Notation	n(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		
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		



$$m = 0, -1, +1$$
$$s = +\frac{1}{2}, -\frac{1}{2}$$