VE320 – Summer 2022

Introduction to Semiconductor Devices

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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

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2.6 Electrons in an atom

2.1 2^{nd} order differential equations and waves

k real k^2 positive

$\frac{d^2y}{dx^2} = k^2 y$	General solution: $y = Ae^{bx}$
$\frac{dy}{dx} = A \cdot b e^{bx}$ $\quad \frac{d^2y}{dx^2} = A \cdot b^2 \cdot e^{bx}$	
$\cancel{A} \cdot b^2 \cdot \cancel{e^{bx}} = k^2 \cdot \cancel{A}\, \cancel{e^{bx}}$	
$y = A_1 e^{kx} + A_2 e^{-kx}$	
$\frac{d^2y}{dx^2} = -k^2 y$	General solution: $y = Ae^{bx}$
$\cancel{Ab^2e^{bx}} = -k^2 \cdot \cancel{Ae^{bx}}$	
$y = A_1 \cdot e^{ikx} + A_2 e^{-ikx}$	

$A_1 e^{kx}$, $A_2 e^{-kx}$

$b^2 = k^2$

$b = \pm k$

$b^2 = -k^2$

$b = \pm i \cdot k$

2.1 2nd order differential equations and waves

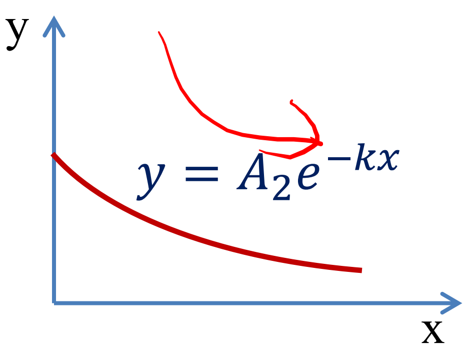
$$\frac{\partial^2 y}{\partial x^2} = k^2 y$$

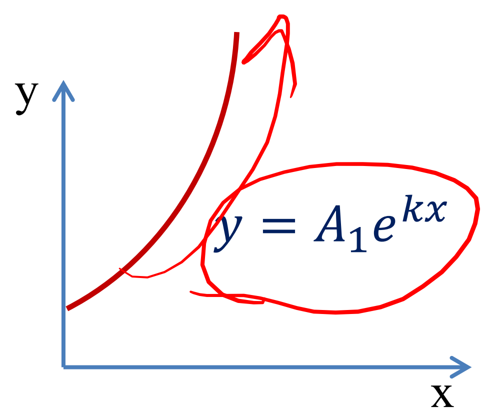
General solution: $y = Ae^{bx}$

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

$$\Rightarrow b = \pm k$$

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

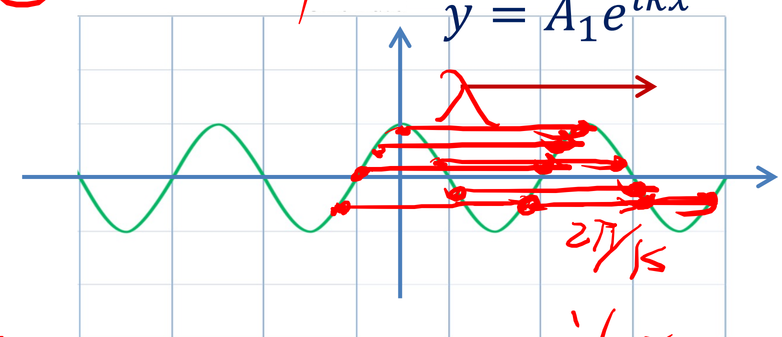


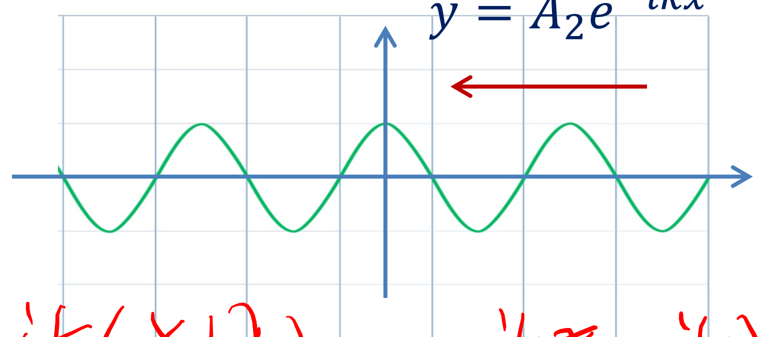


2.1 2nd order differential equations and waves

$k \cdot \lambda = 2\pi$ $\quad \lambda = \frac{2\pi}{k} =$ wavelength

$e^{i2\pi} = 1$





$e^{ik\lambda} = 1$ $\quad e^{ikx} = e^{ik(x+\lambda)} = e^{ikx} \cdot e^{ik\lambda}$

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

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

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

$$\Rightarrow b = \pm ki$$

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

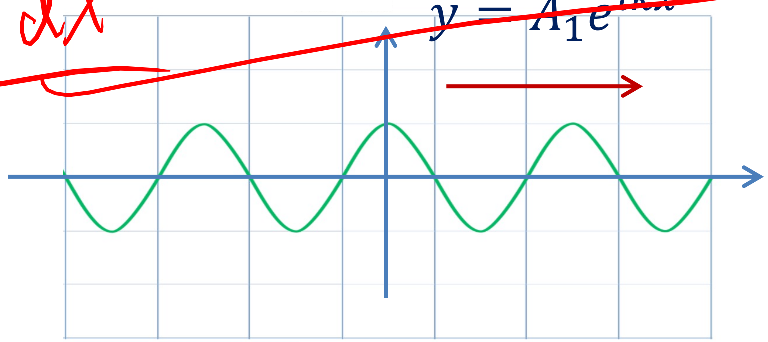
$k =$

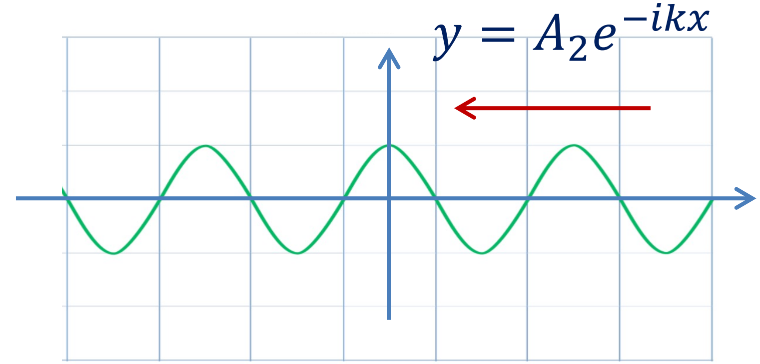
e^{ikx}

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

2.1 2nd order differential equations and waves

$$\frac{d^2y}{dx^2} = -\left(\frac{2\times3.14}{1\times10^{-6}}\right)\cdot y^2$$





$\lambda_0 = \lambda = 1\,\mu m$

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.

$$\frac{d^2y}{dx^2} = -k^2\cdot y$$

$$\boxed{\frac{d^2y}{dx^2} = -\left(\frac{2\pi}{\lambda_0}\right)\cdot y}$$

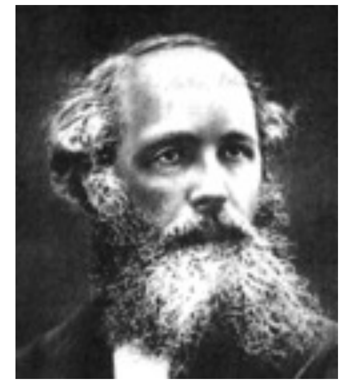
1×10^{-6}

$$\lambda_0 = \frac{2\pi}{k} \Rightarrow k = \frac{2\pi}{\lambda_0}$$

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

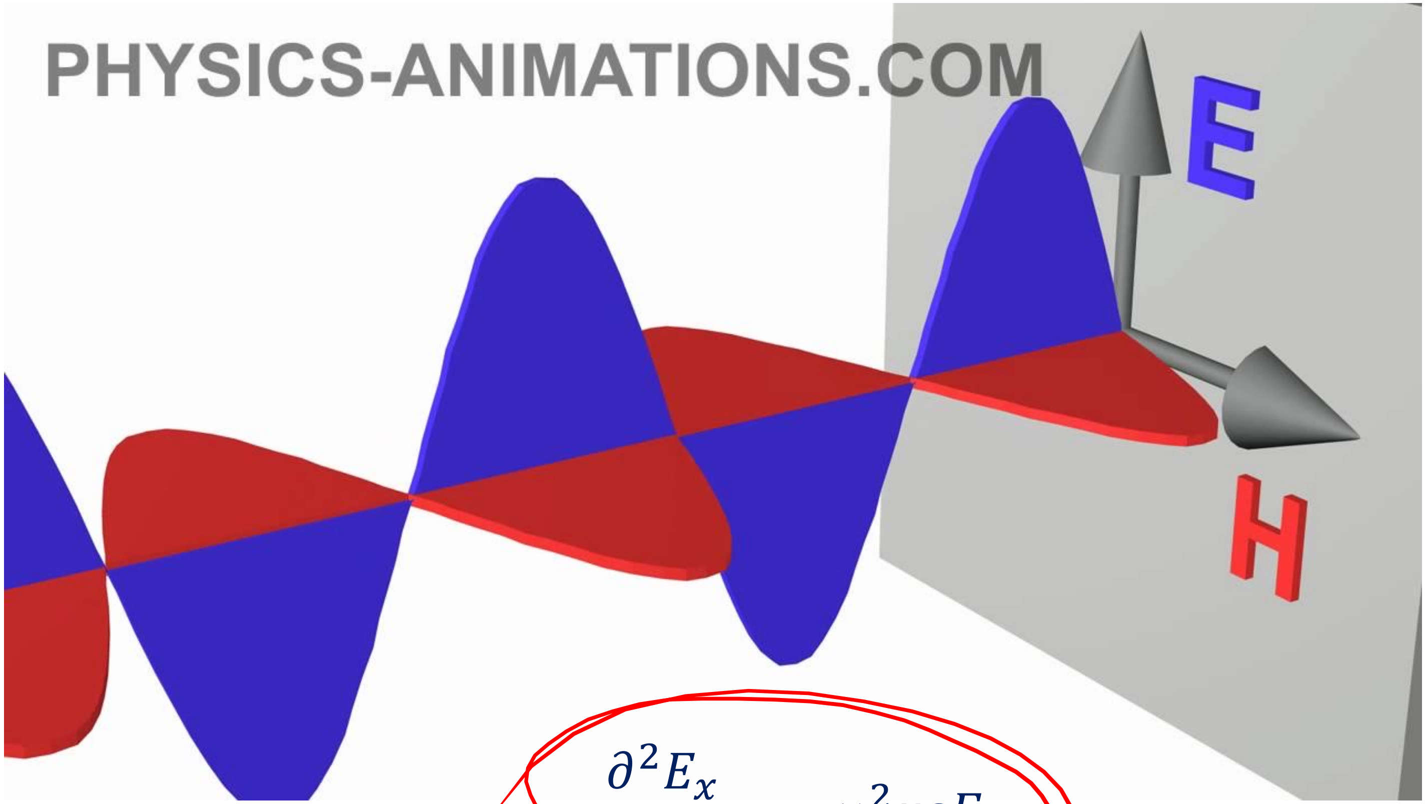
Static differential equation describing the electromagnetic wave

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

solution is wave

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

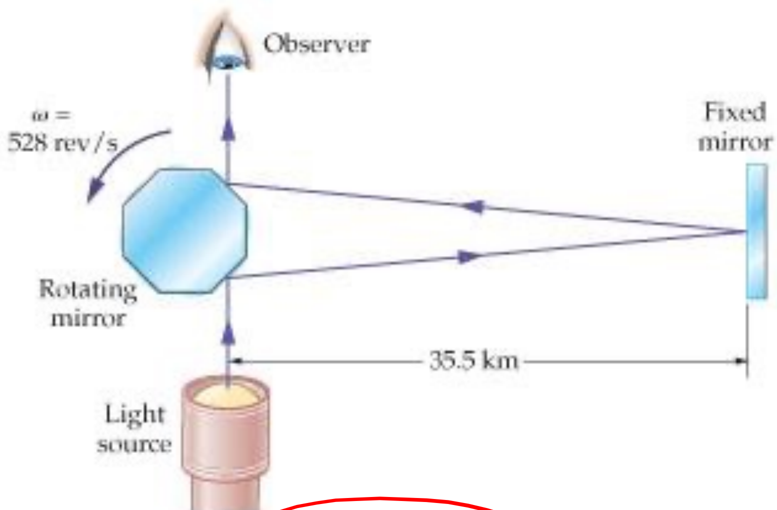
2.4 Electrons in infinite quantum well

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 $v = 2.98\times10^8 m/s$



Rotation mirror

Leon Foucault

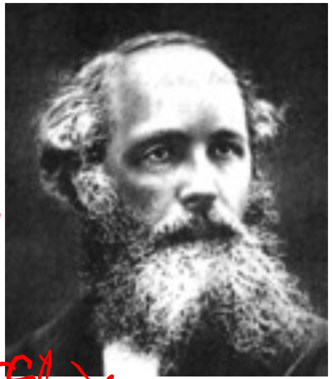
2.2 Historic events in developing quantum mechanics

② Maxwell Equations in the year 1865

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

light - wave

electromagnetic wave



James Maxwell

Static differential equation describing the electromagnetic wave $e^{i\omega t}$

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

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

$\sqrt{\mu\varepsilon}\cdot x = t$

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

$v = \frac{x}{t} = \frac{1}{\sqrt{\mu\varepsilon}}$

Light is an electromagnetic wave!

2.2 Historic events in developing quantum mechanics

③ Light wave-particle duality in 1905

deep UV light

green

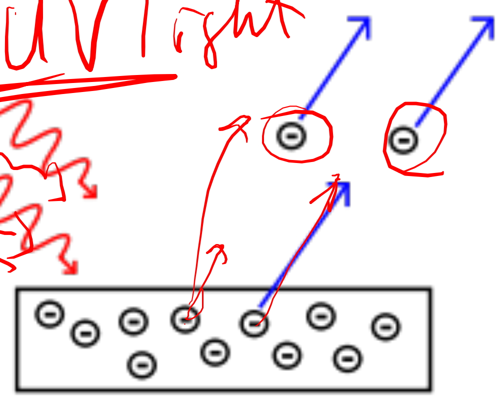
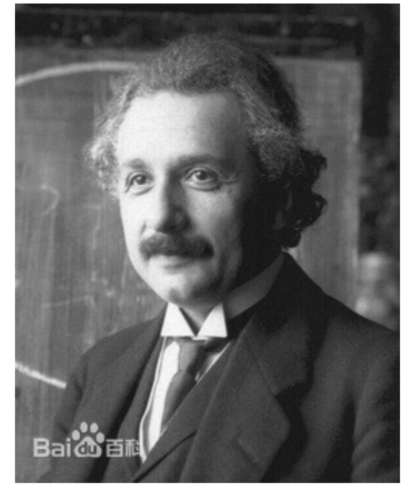


Photo-electric experiment



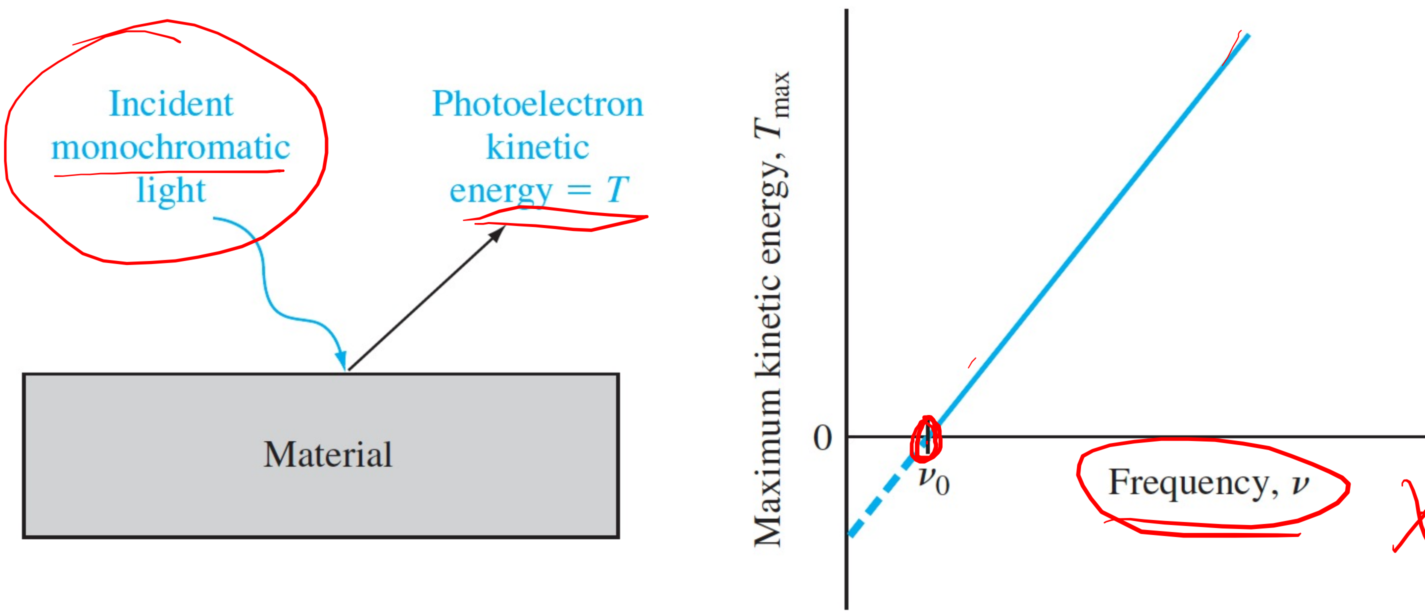
Albert Einstein
Nobel Prize 1921

- ❑ 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

λ_0



λ_0

(a) (b)

- Light wave is a particle: $h\nu = K_{max} + W_c$

③ Light wave-particle duality in 1905

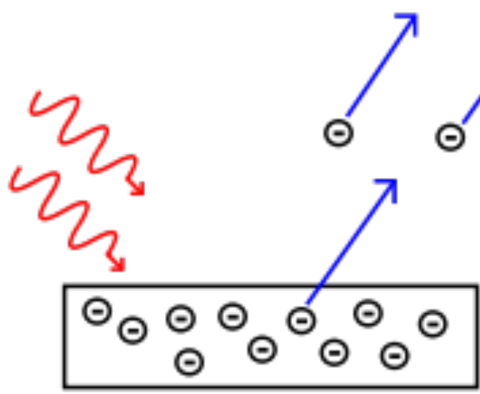
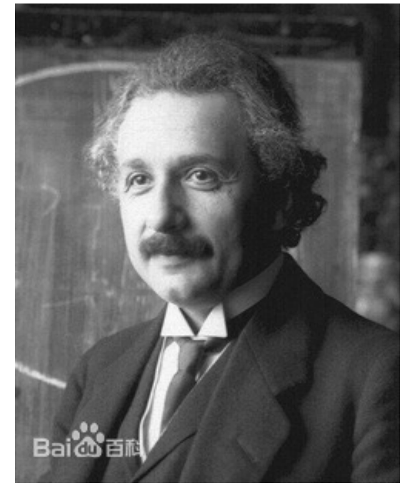


Photo-electric experiment



Albert Einstein
Nobel Prize 1921

f

$2\pi f = \omega$

$$E = h\nu = \hbar\omega \qquad E = mc^2$$

momentum

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

$\boxed{\text{Light is a particle!}}$

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

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

2.2 Historic events in developing quantum mechanics

④ Matter wave hypothesis in 1924

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

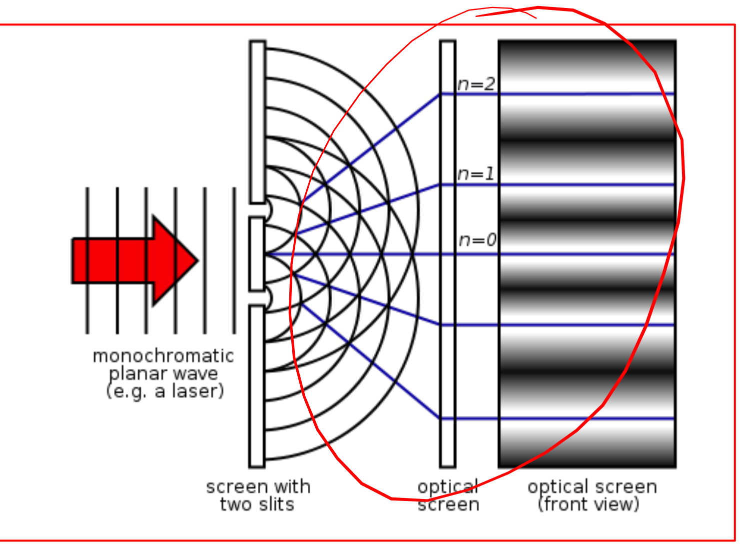
$p = m \cdot v \Rightarrow p = \hbar k$

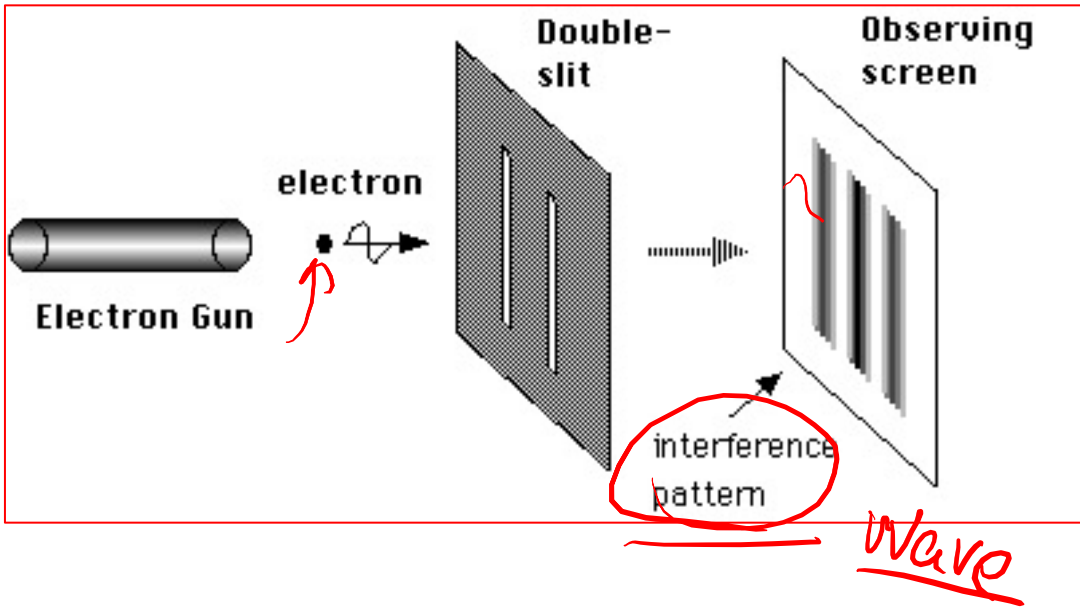
Louis Victor de Broglie
Nobel Prize 1929

$k = \frac{2\pi}{\lambda}$ wavenumber λ wavelength

2.2 Historic events in developing quantum mechanics

④ Matter wave hypothesis in 1924





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2.3 A case study

$$\frac{\partial^2 y}{\partial x^2} = -k^2 y \qquad v = \sqrt{\frac{2eV_0}{m_0}}$$

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

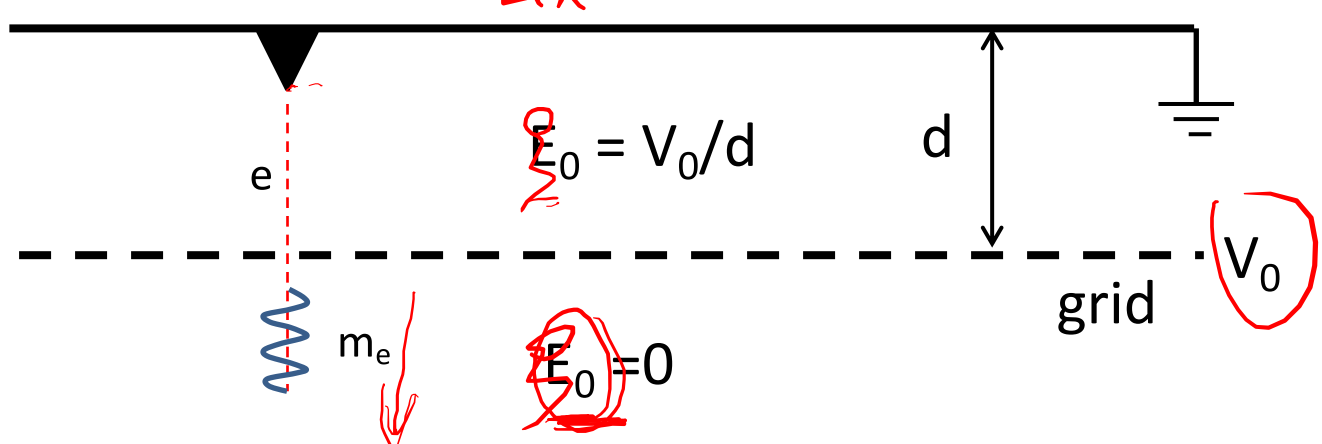
$$E = \frac{1}{2}mv^2 = e \cdot V_0 = E = h\text{v} = \hbar\omega$$

$$\text{p} = mv_0 = \text{p} = \frac{h}{\lambda} = \hbar k$$

$$k = \frac{2\pi}{\lambda_0}$$

Quiz #1:

$$\frac{d^2 y}{dx^2} = -k^2 \cdot y$$



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

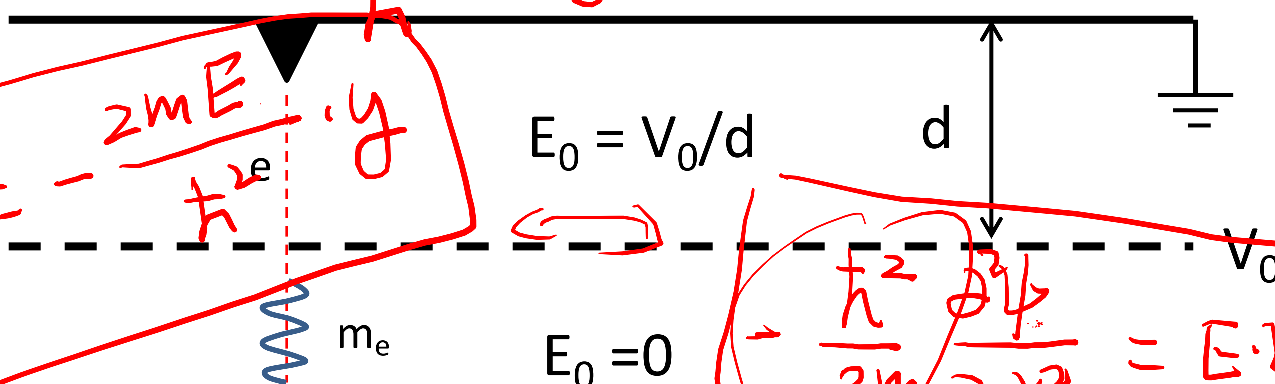
2.3 A case study

$$\frac{1}{2} m_0 v_0^2 = eV_0 \Rightarrow v_0 = \sqrt{\frac{2eV_0}{m_0}}$$

$$p = m_0 \cdot v_0 = \hbar k \Rightarrow k = \frac{m_0 \cdot v_0}{\hbar} = \frac{m_0 \sqrt{\frac{2eV_0}{m_0}}}{\hbar} = \frac{\sqrt{2eV_0 m_0}}{\hbar}$$

$$\frac{d^2y}{dx^2} = -\frac{2eV_0 m_0}{\hbar^2} \cdot y$$

$$\boxed{\frac{d^2y}{dx^2} = -\frac{2mE}{\hbar^2} \cdot y}$$



$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = E \cdot \psi}$$

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

2.3 A case study

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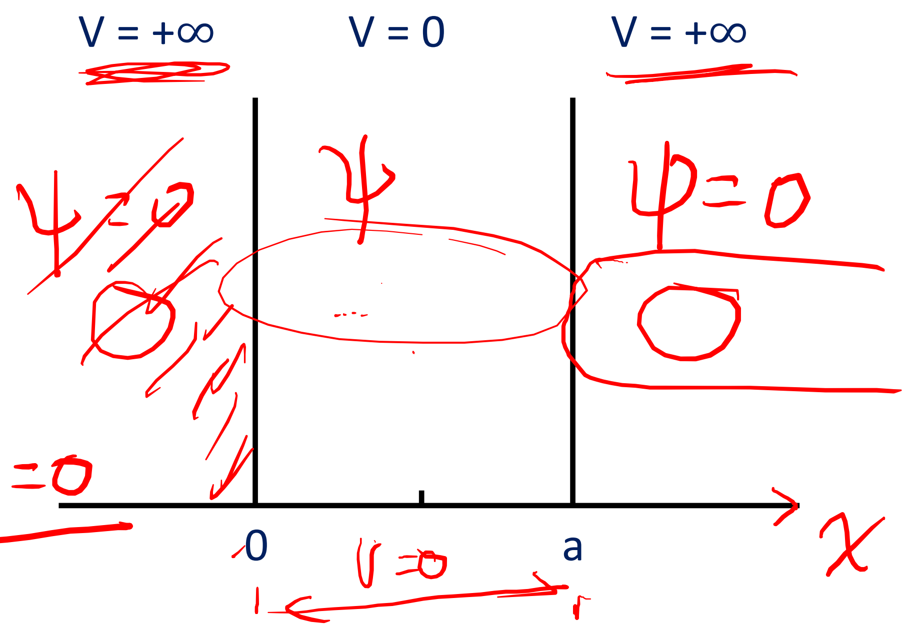
2.4 Electrons in Infinite Quantum Well

$\nearrow +\infty$ $\quad \psi = 0$

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



Conditions:

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

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

$for\ 0 < x < a$

$V(x) = 0$

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

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

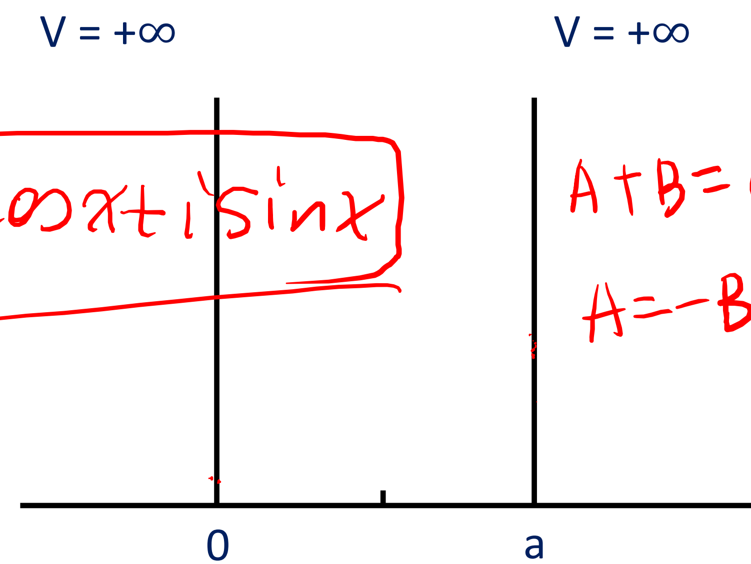
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\cdot\psi = -k^2\psi$

$\psi = A\cdot e^{-kx} + Be^{kx}$ $\quad k = \pm\frac{\sqrt{2mE}}{\hbar}$

2.4 Electrons in Infinite Quantum Well

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

$e^{ix} = \cos x + i\sin x$



$A + B = 0$

$A = -B$

Conditions:

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

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

$for\ 0 < x < a$

$V(x) = 0$

$x = 0\ \ \psi(0) = 0 \qquad x = a\ \ \psi(a) = 0$

$\psi(x)\big|_{x=0,a} = 0$

$x=0\ \ \psi(x) = Ae^{-ik0} + Be^{ik0} = 0$

$x=a\ \ \psi(a) = Ae^{-ika} + Be^{ika} = 0$

$-B(\cos ka - i\sin ka) + B(\cos ka + i\sin ka) = 0$

2.4 Electrons in Infinite Quantum Well

$$\begin{cases} A(\cos ka - i\sin ka) + B(\cos ka + i\sin ka) = 0 \\ A = -B \end{cases}$$

$$\Rightarrow -B(\cos ka - i\sin ka) + B(\cos ka + i\sin ka) = 0$$

$$-B\cos ka + iB\sin ka + B\cos ka + iB\sin ka = 0$$

$$\boxed{2iB\sin ka = 0}$$

$0, \pm 1, \pm 2$

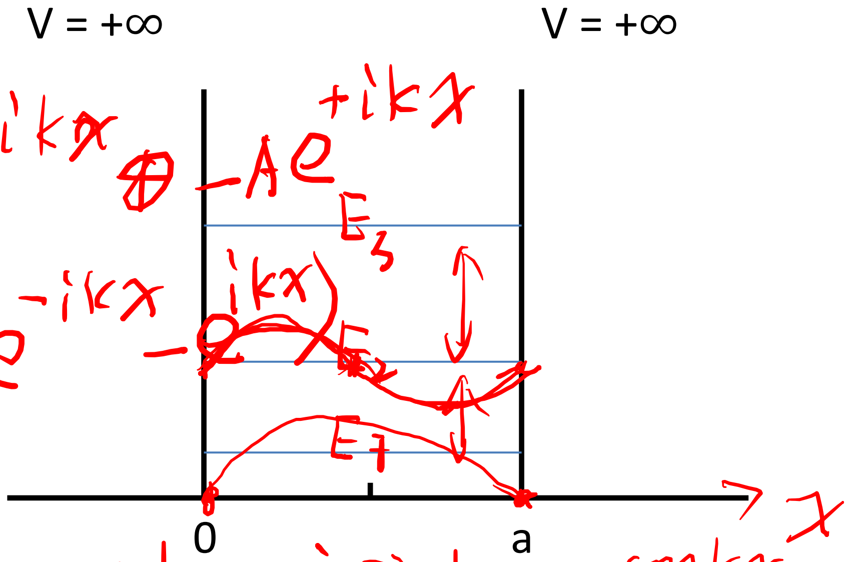
n: integer

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

$$ka = n\cdot\pi \Rightarrow \boxed{k = \frac{n\cdot\pi}{a}}$$

2.4 Electrons in Infinite Quantum Well

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



$\psi(x) = A e^{-ikx} - A e^{+ikx}$

$= A(e^{-ikx} - e^{ikx})$

$= A(\cos kx - i\sin kx - \cos kx - i\sin kx)$

$= A(-2i\sin kx)$

Conditions:

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

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

$for\; 0 < x < a$

$V(x) = 0$

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

$n = 0, \pm1, \pm2$

$n=1$ $\quad \psi(x) = -2iA\sin(\frac{\pi}{a}x)$

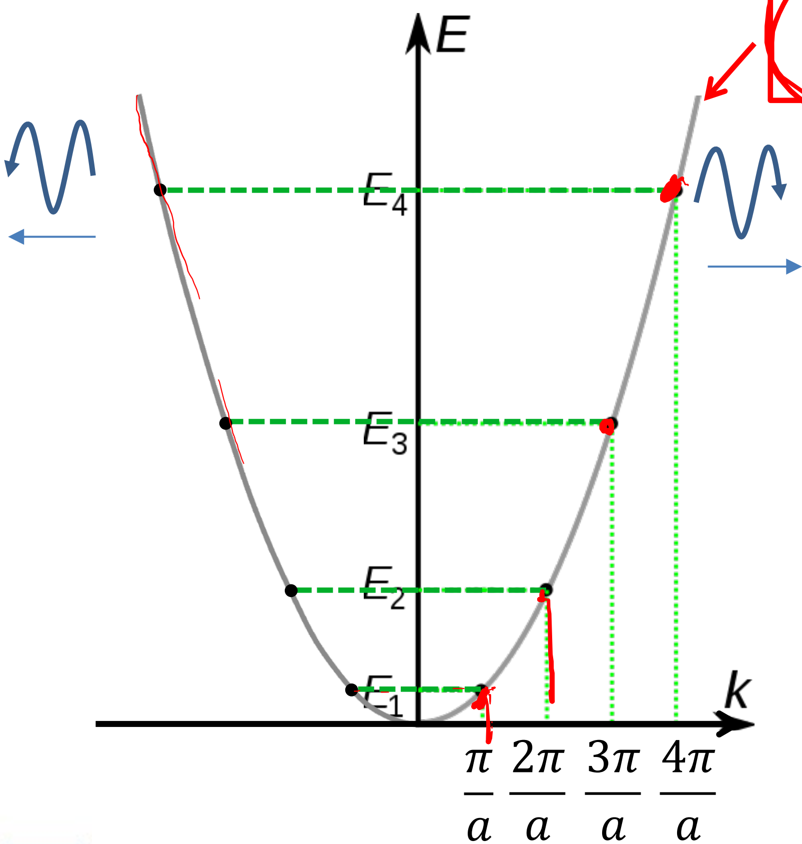
$n=2$ $\quad \psi(x) = -2iA\sin(\frac{2\pi}{a}x)$

$k = \frac{n\pi}{a}$

2.4 Electrons in Infinite Quantum Well

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

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



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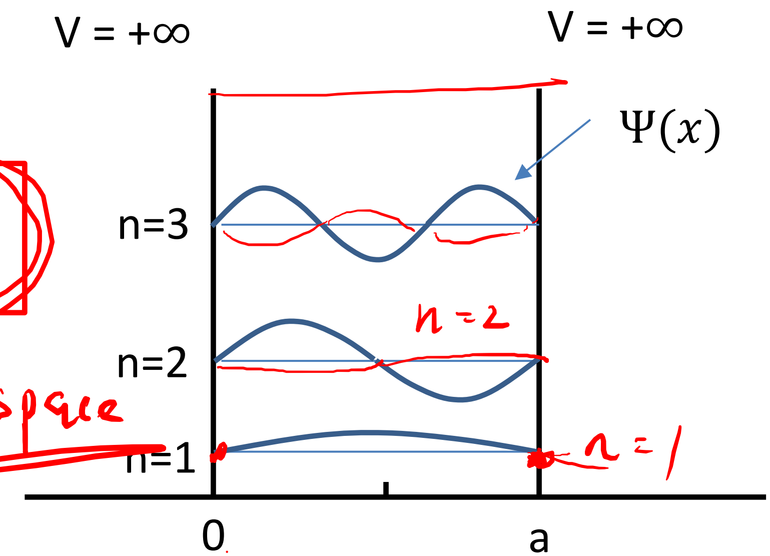
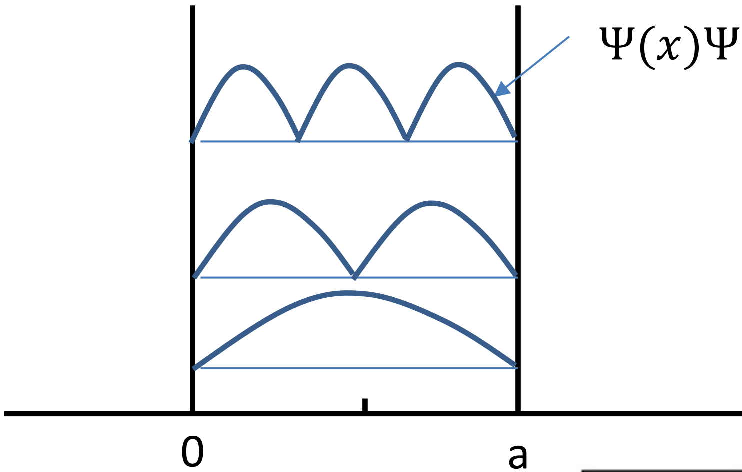


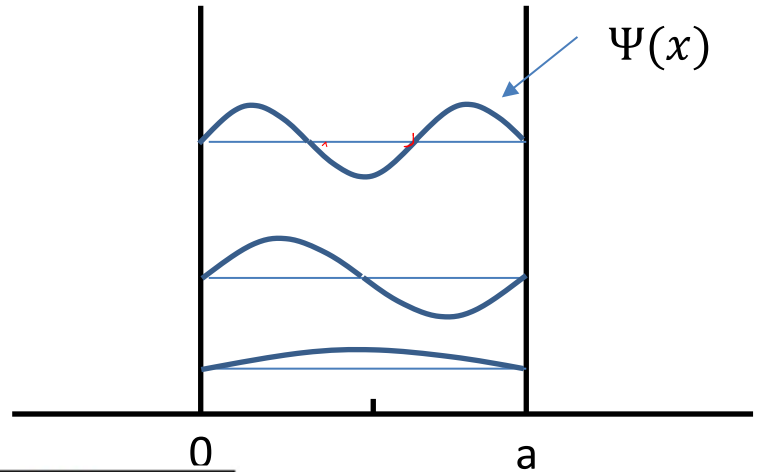
K = ±

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

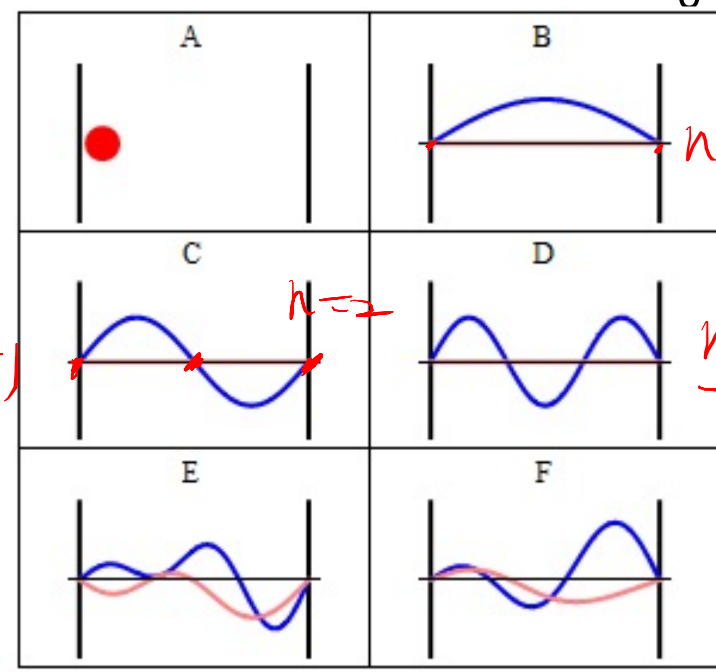
$$k=\frac{n\pi}{a}\qquad n=0,\pm 1,\pm 2,\ldots$$

2.4 Electrons in Infinite Quantum Well





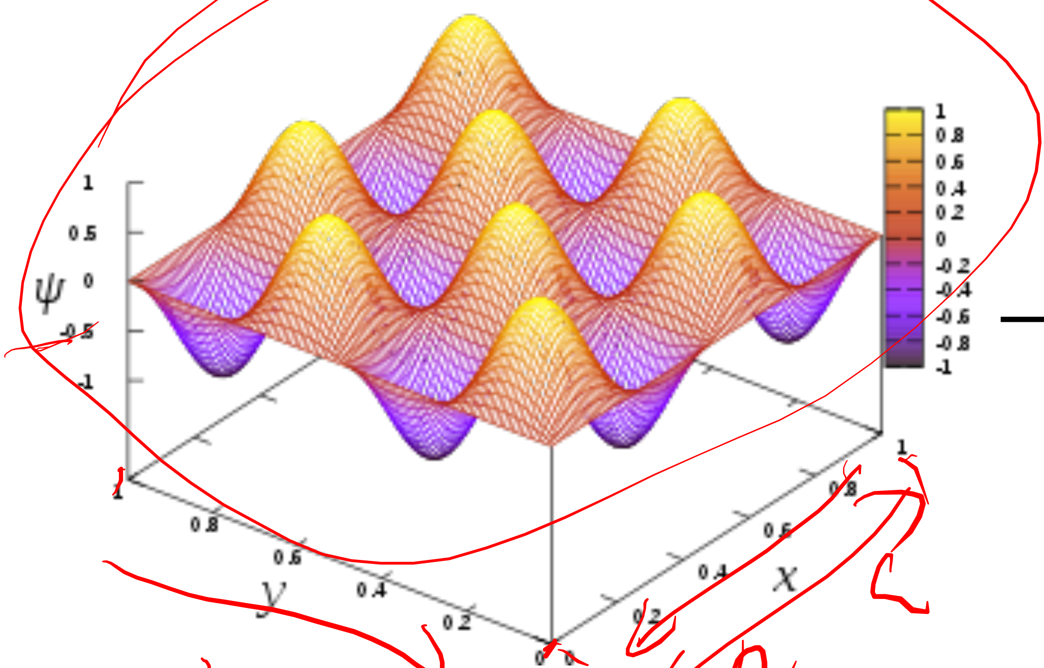
$\psi(x)$



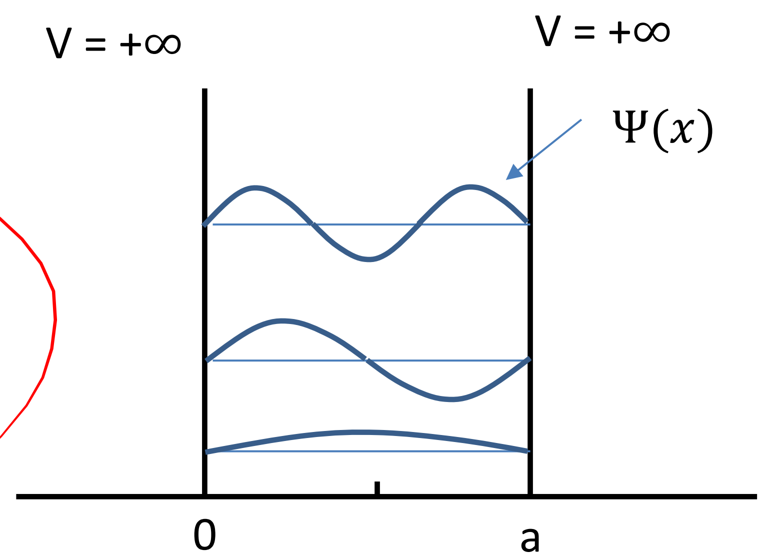
$\psi(x) = Ae^{-ikx} + Ae^{ikx}$

2.4 Electrons in Infinite Quantum Well

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



6 2-dimentional Quantum well



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

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

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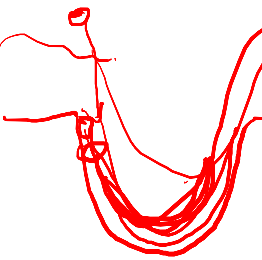
2.5 Electrons in Finite Quantum Well

potential energy

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



Conditions:

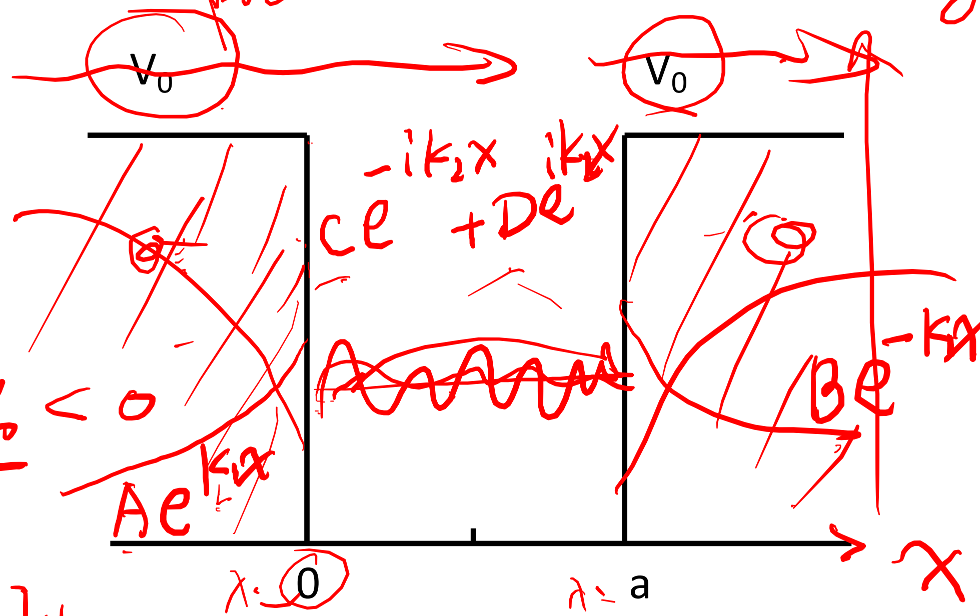
$for\ x \leq 0, x \geq a$

$$V(x) = V_0;$$

$for\ 0 < x < a$

$$V(x) = 0$$

$E - V_0 < 0$



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

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

k^2

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

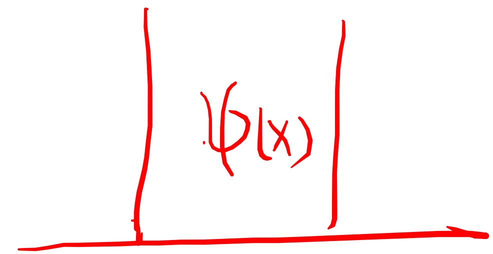
$$\psi(x) = Ae^{kx} + Be^{-kx}$$

$$k = \pm\frac{\sqrt{2m(E-V_0)}}{\hbar}$$

$$k = \pm\frac{\sqrt{2m(V_0-E)}}{\hbar}$$

2.5 Electrons in Finite Quantum Well

$0 < x < a \qquad V(x) = 0$



$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \overset{=0}{V(x)}\cdot\psi = E\cdot\psi$$

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

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

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

$$\psi(x) = C\cdot e^{-ikx} + De^{+ikx}$$

2.5 Electrons in Finite Quantum Well

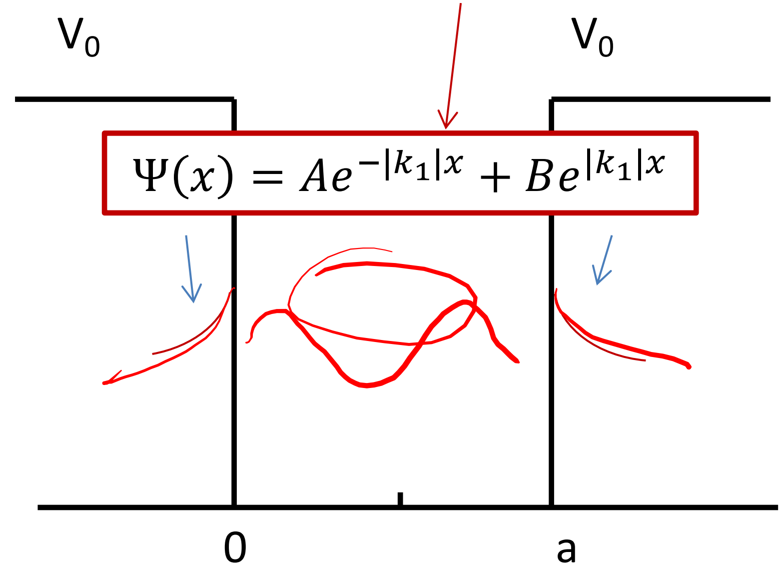
If E < V_0 $\quad k_1 = i\sqrt{\dfrac{2m(V_0 - E)}{\hbar^2}}$

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:

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

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

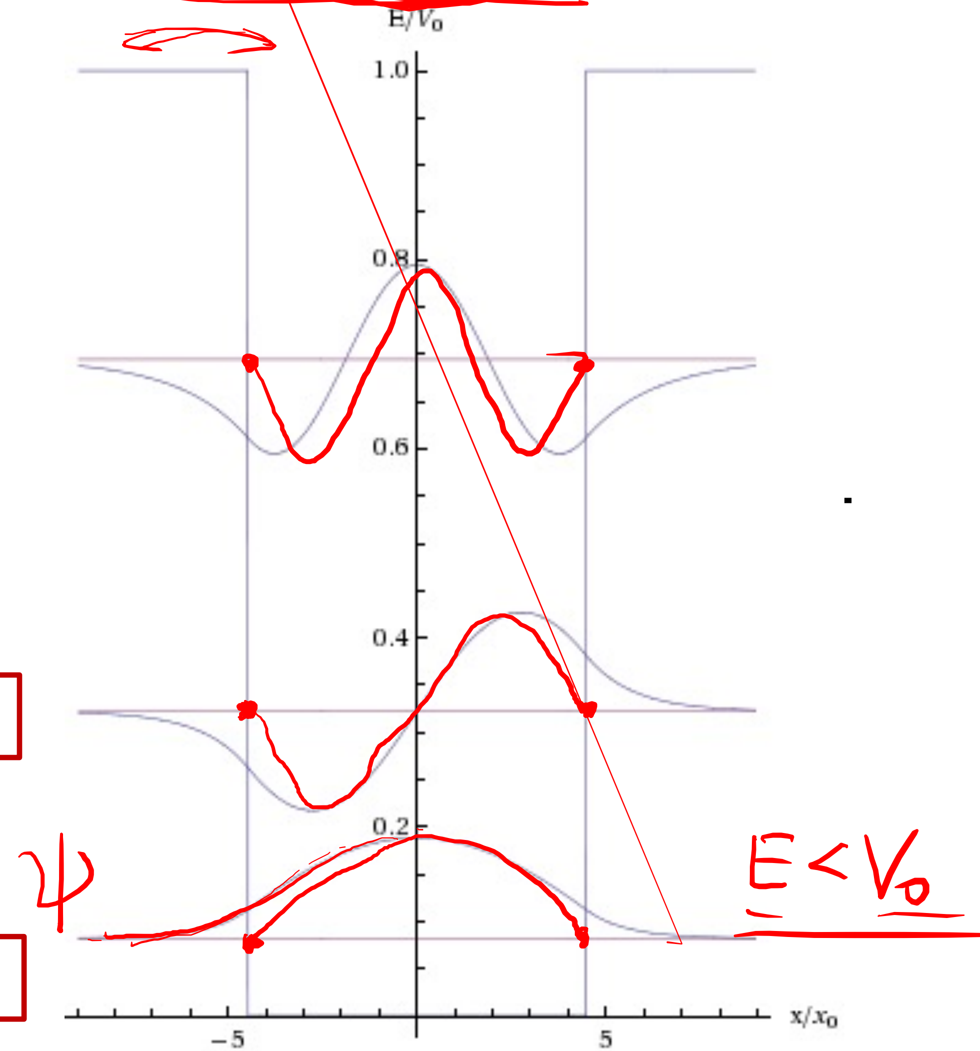
$$\int_{-\infty}^{\infty}\Psi(x)\Psi^{*}(x)dx = 1$$

$for\ x < 0, x > a$

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

$for\ 0 \le x \le a$

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



Outline

2.1 2^{nd} order differential equations and waves

2.2 Historic events in developing quantum mechanics

2.3 A case study

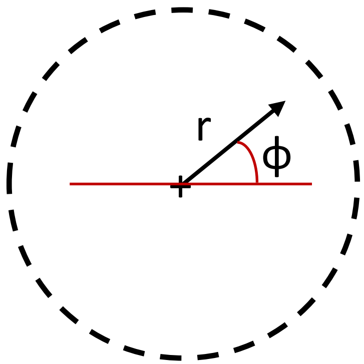
2.4 Electrons in infinite quantum well ideal solve

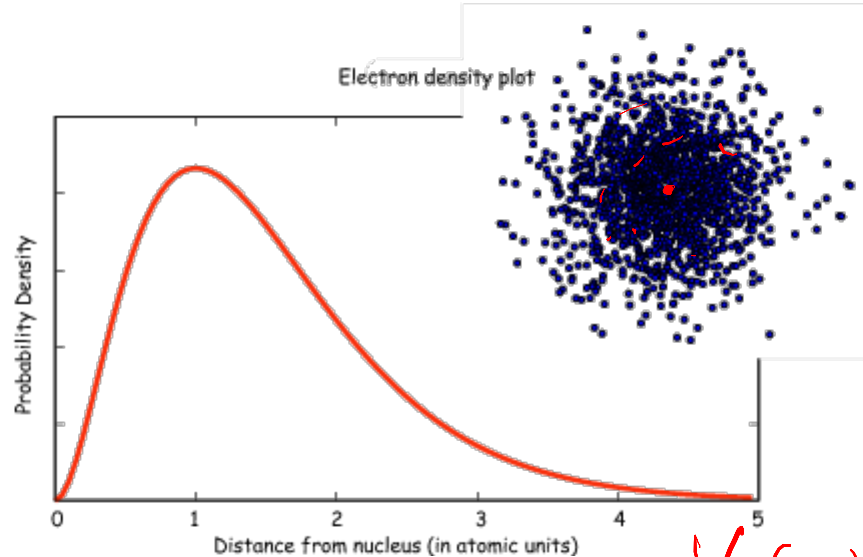
2.5 Electrons in finite quantum well less ideal

2.6 Electrons in an atom

2.6 Electrons in an Atom

- 2D



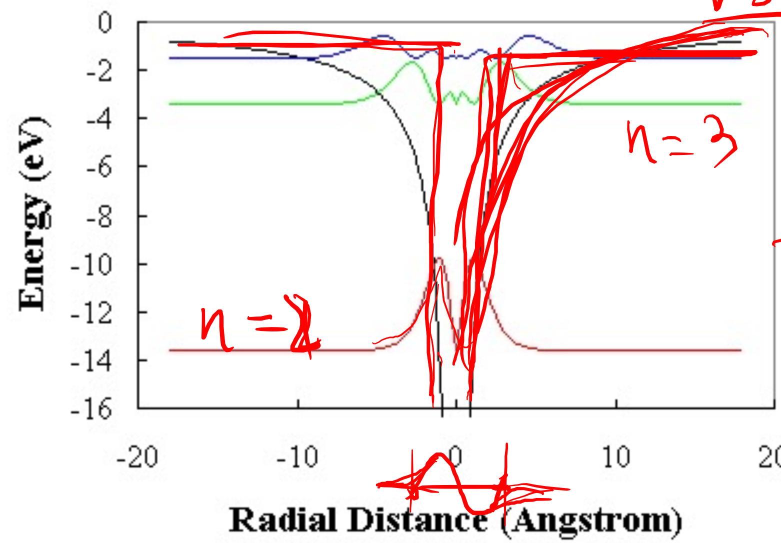


Periodic boundary conditions

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

$$\frac{e}{x}$$

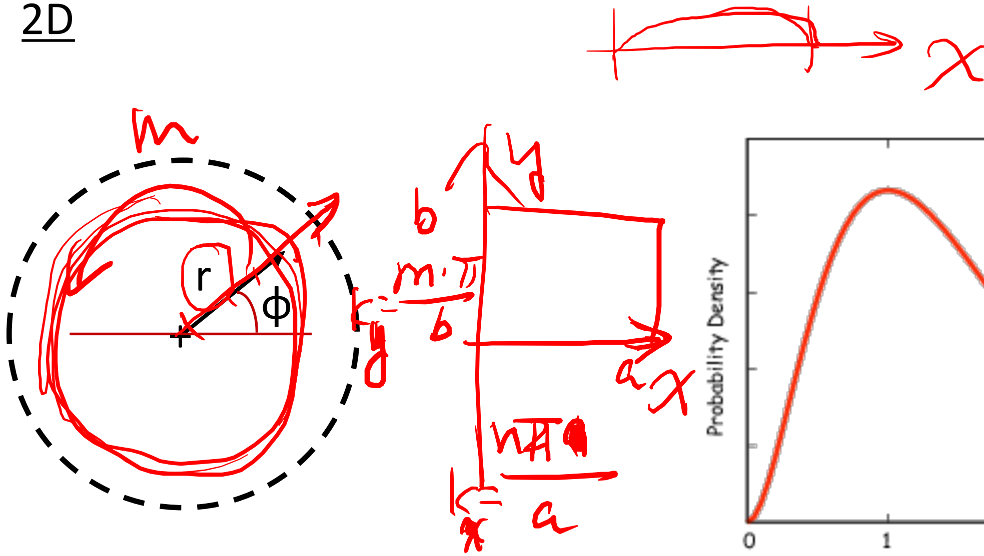
$$\frac{V_0(x)\approx\frac{q}{x}}{V_0}$$

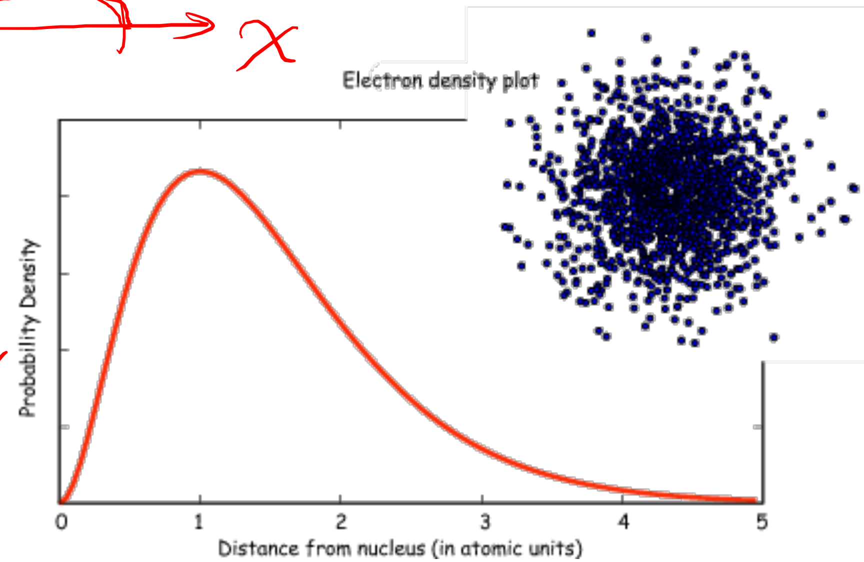


$$\frac{\psi\cdot\psi^*=P}{\psi}$$

2.6 Electrons in an Atom

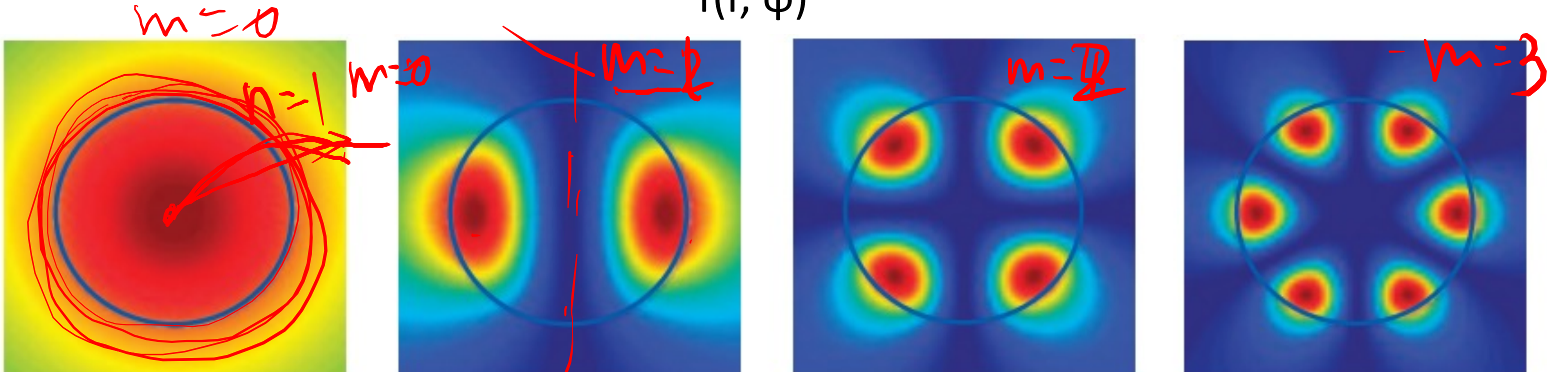
- 2D





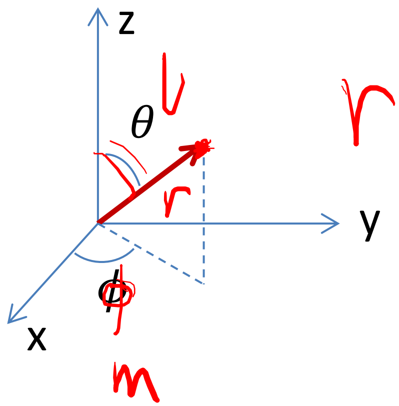
Periodic boundary conditions

f(r, ϕ)



2.6 Electrons in an Atom

- 3D

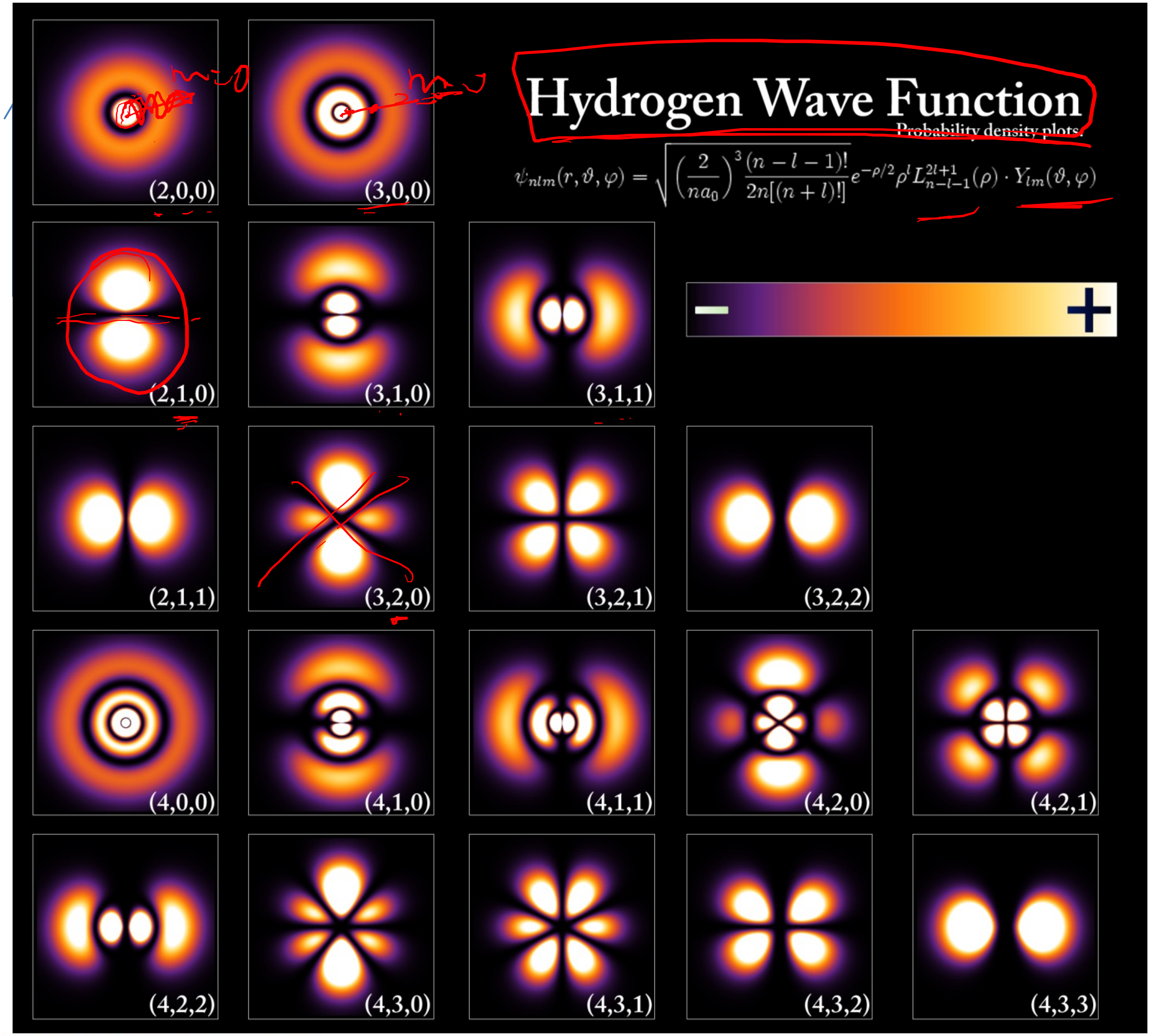


r n

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

2.6 Electrons in an Atom

- 3D



$3s^2 3p^6 3d^6$
$2s^2 2p^6$
$1s^2$

n

n m

2.6 Electrons in an Atom

- 3D

Schringo

spin

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		