Photons, Waves, Tunneling, Particle Boxes

Wednesday, November 4, 2020 6:04 PM

Electrons / Photons

- Electromagnetic Radiation → particles = photons
- E photon ∝ freq & momentum ∝ 1/wavelength

$E = h\nu$ $c = \nu\lambda$

$h\nu$ → photon Energy

Photoelectric Effect

- light's photon sufficient to eject e^-
- Transfers energy → needs minimum energy: work function

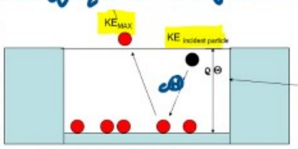
Wavelength: Long → No Emission e^-, even @ ↑f
Short → Emission e^-, even @ ↓f

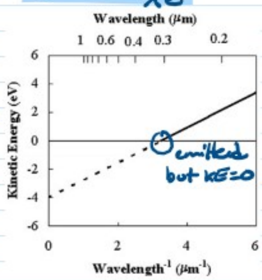
Kinetic Energy & Work Function

- E of e^- ejected ∝ light freq.

$KE = h\nu - e\Theta$ → $e\Theta$ = min. E to extract e^-
Θ = work function (eV)

$\underbrace{h\nu}_{\text{photon Energy}} = \underbrace{Vq}_{\text{current } q=-e} + \underbrace{e\Theta}_{\text{energy to eject}}$ → $\Theta = \frac{h\nu}{e} + V = \frac{hc}{\lambda e}$ → $\Theta = q\varphi_m$





$KE_{max} = KE_{\text{incident particle}} - e\Theta$

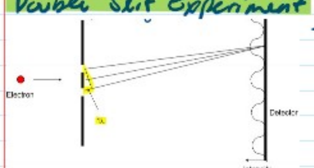
↳ Energy of Ejected e^-

- Momentum: $p = \frac{h}{\lambda}$
- Visible light: 400nm — 700nm → photons 1.7–3.2eV
- Conversion: $1eV = 1.60218 \times 10^{-19}$ J → e^-
- Θ = ~2.1–5.5eV for metals
- Not every photon leads to ejection:
  - If $E_{photon} < e\Theta$ → NO
  - If $E_{photon} \geq e\Theta$ → Maybe, may collide w/ other e^-, not enough E

Electrons as Waves

- Form standing waves → orbitals (atomic, bonding, molecular)
- In solids: waves → Energy levels & bands

Double Slit Experiment



- Constructive Interference
↳ path length differs by $n\lambda$

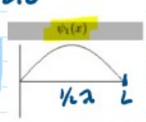
Wave Particle Duality

- e^- has mass & charge but interferes like waves
- De Broglie: $\lambda = \frac{h}{p} = \hbar K$ → $k = \frac{2\pi}{\lambda}$
- Heisenberg Uncertainty principle
  - The better we know e^- position, the worst we know momentum/λ/speed
  $\Delta x \Delta p \geq \hbar/2$ → $\hbar = \frac{h}{2\pi}$ → (planck's const)

- Kinetic Energy for e^- wave:
$KE = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 K^2}{2m}$

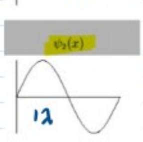
$KE = \frac{\hbar^2}{2m\psi} \cdot \frac{\partial^2\psi}{\partial x^2}$

- 3/2λ has the highest KE
- $E_{Total} = KE + U$ → U = PE
- ↓λ = ↑p & ↑KE



lowest Estate → longest λ allowed = 2L ∵ lowest order λ has sheet length $L = \frac{\lambda}{2}$ & $\psi(x) = 0$ at walls

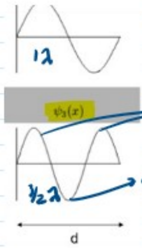
For lowest E λ: $\lambda = 2L$, $k = \frac{2\pi}{\lambda}$, $\psi(x) = A\sin\left(\frac{\pi x}{L}\right)$
In 3D: $\psi(x) = A_x\sin\left(\frac{\pi x}{L}\right) A_y\sin\left(\frac{\pi y}{L}\right) A_z\sin\left(\frac{\pi z}{L}\right)$



2nd Estate

Shrödinger's Equation

- $E_{total} = KE + U \rightarrow U = PE$ ... and state
- $\downarrow \lambda = \uparrow p$ & $\uparrow KE$



Shrödinger's Equation

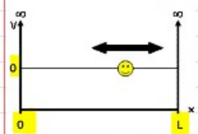
1D: $j\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + U\psi$

$\underbrace{j\hbar \frac{\partial \psi}{\partial t}}_{\text{Total } E}$, $\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}}_{KE}$, $\underbrace{U\psi}_{PE}$

1D Particle Box

- particle moving horizontally in infinit well
- Solutions: $E \rightarrow$ Allowed Energy
  $\psi(x) \rightarrow$ wave function, when squared = probability of locating e- @ x at given E level

① Define Potential Energy V



- Particle in ∞ Potential well length L
- $PE = V = U = 0$ in box $V = 0$ for $0 < x < L$
- $V = \infty$ for $x < 0$ or $x > L$
  ↳ Boundary conditions, $U = \infty$ @ walls

② Solve Shrodinger's Equation

- For particle mass m moving w/ Energy E:

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) \xrightarrow{V(x)=0} E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}$$

↳ General Soln: $\psi(x) = A\sin(kx) + B\cos(kx)$

③ Define wave function

- Apply Boundary conditions: @ $x = 0$ or $L = 0$, $\sin(0) = 0$ & $\cos(0) = 1$, $\psi(x) = 0$

→ solve for k: $k = \left(\frac{8\pi^2 mE}{h^2}\right)^{1/2}$ $\therefore B = 0$, $\psi(x) = A\sin(kx)$ ↳ $k = \frac{2\pi}{\lambda}$

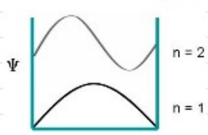
$\therefore \psi = A\sin\left(\frac{8\pi^2 mE}{h^2}\right)^{1/2} x$

→ solve for A: use Boundary conditions $x = L \rightarrow \psi(x) = 0$

$\left(\frac{8\pi^2 mE}{h^2}\right)^{1/2} L = n\pi$

$\therefore \psi = A\sin\left(\frac{n\pi}{L}\right)x$ → Normalize wave function: $\int_0^L \psi^2 dx = 1 \rightarrow A = \sqrt{\frac{2}{L}}$

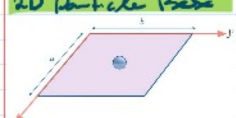
$\therefore \psi = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}\right)x$



④ Allowed Energies

$E_n = \frac{n^2 h^2}{8mL^2}$

2D Particle Box

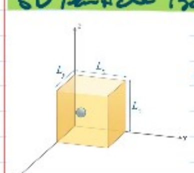


- Boundary Conditions: $0 < x < a$, $0 < y < b$
  $V(x,y) = 0$ & $\psi(x,y,t) = 0$ @ walls
- Shrödinger Eqn 2D: $E\psi(x,y) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2}\right) + V(x,y)\,\psi(x,y)$
  $\because V(x,y) = 0$ $\therefore E\psi(x,y) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2}\right)$ $\psi(x,y) = \psi_x(x)\psi_y(y)$
- General Soln: $\psi_x(x) = A_x\sin(k_x x) + \cancel{B_x\cos(k_x x)}$
  $\psi_y(y) = A_y\sin(k_y y) + \cancel{B_y\cos(k_y y)}$

$\psi(x,y) = N\sin\left(\sqrt{\frac{2mE_x}{\hbar^2}}\,x\right)\sin\left(\sqrt{\frac{2mE_y}{\hbar^2}}\,y\right) = N\sin\left(\frac{n_x\pi x}{L}\right)\sin\left(\frac{n_y\pi y}{L}\right)$ → normalize: $N = \frac{2}{L}$

- Allowed Energy: $E_{n_x n_y} = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2)$

3D Particle Box



- Boundary Conditions: $0 \leq x \leq L_x$, $0 \leq y \leq L_y$, $0 \leq z \leq L_z$
- $V(\vec{r}) = 0$ potential in box → $\vec{r} = L_x\hat{x} + L_y\hat{y} + L_z\hat{z}$

$E\psi(r) = -\frac{\hbar^2}{2m}\left(\frac{d^2\psi(r)}{dx^2} + \frac{d^2\psi(r)}{dy^2} + \frac{d^2\psi(r)}{dz^2}\right)$ $\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z)$

→ normalized: $\psi(r) = \sqrt{\frac{8}{L^3}}\sin\left(\frac{n_x\pi x}{L_x}\right)\sin\left(\frac{n_y\pi y}{L_y}\right)\sin\left(\frac{n_z\pi z}{L_z}\right)$ → normalize: $A_x = A_y = A_z = \sqrt{\frac{2}{L}}$

- Allowed Energy: $E_{n_x n_y n_z} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right) = KE$

@ ground state (lowest E): $KE_{111} = \frac{3h^2}{8mL^2}$ → Total $E = KE + U_0$ (potential E)

- Degeneracy: - @ ground state → 1 wave function $\therefore$ non-degenerate → (1, 1, 1)
  - If has >1 states/wave func. $\therefore$ degenerate

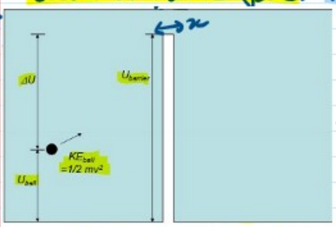
@ ground state (lowest E): $KE_{1,1,1} = \frac{3h^2}{8mL^2}$

- Degeneracy: - @ ground state → 1 wave function ∴ non-degenerate → (1,1,1)
  - If has >1 states/wave func. ∴ degenerate
    ↳ Sum of squares of quantum numbers = same → $n^2 = n_x^2 + n_y^2 + n_z^2$
  - # wavefunc. = degree of degeneracy of energy level
  - n^2 = coeff. to multiply $\frac{h^2}{8mL^2}$

$n_x^2+n_y^2+n_z^2$	Combinations of Degeneracy (n_x, n_y, n_z)			Total Energy (E_{n_x,n_y,n_z})	Degree of Degeneracy
3	(1,1,1)			$\frac{3h^2}{8mL^2}$	1
6	(2,1,1)	(1,2,1)	(1,1,2)	$\frac{6h^2}{8mL^2}$	3
9	(2,2,1)	(1,2,2)	(2,1,2)	$\frac{9h^2}{8mL^2}$	3
11	(3,1,1)	(1,3,1)	(1,1,3)	$\frac{11h^2}{8mL^2}$	3
12	(2,2,2)			$\frac{12h^2}{8mL^2}$	1

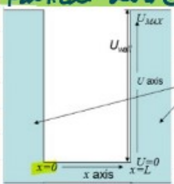
Tunneling
- ↓ Transistor size → tunneling b/w gate channel, energy leakage
- Consequence of wave nature of e^-
  ↳ "leaks" into regions they don't have enough E to be in
- Soln. of wave func: $\Psi(x) = Ae^{\sqrt{\frac{2m}{\hbar^2}(U-E)}x} + Be^{-\sqrt{\frac{2m}{\hbar^2}(U-E)}x}$

U



- Potential E: U = mgh
- KE = ½ mv²
- If enough U, go over "barrier"
- ↓x = ↓ probability that e^- in well
  ↳ If narrow, e^- may leak through or divide across both sides

Particle inside Potential well

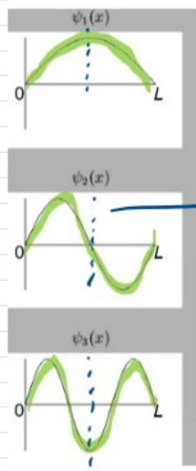


U > E: $\Psi(x) = Ae^{\sqrt{\frac{2m}{\hbar^2}(U-E)}x} + Be^{-\sqrt{\frac{2m}{\hbar^2}(U-E)}x}$

- For $x > L$: $A = 0$ ∴ $\Psi(x) = Be^{-\sqrt{\frac{2m}{\hbar^2}(U-E)}x}$

  $x < 0$: $B = 0$ ∴ $\Psi(x) = Ae^{\sqrt{\frac{2m}{\hbar^2}(U-E)}x}$

- As $U \to \infty$, $\Psi \to 0$



mean position of state

- Infinite Potential Well: $U_{max} \to \infty$

Soln. in well when U=0: $\Psi(x) = Ae^{i\sqrt{\frac{2m}{\hbar^2}E}x} + Be^{-i\sqrt{\frac{2m}{\hbar^2}E}x}$
↳ Boundary conditions: Ψ=0 @ x=0, $U_{max} \to \infty$ @ x=L

@ x=0, B=−A, 1=0 or $\Psi(x) = A'\sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right)$

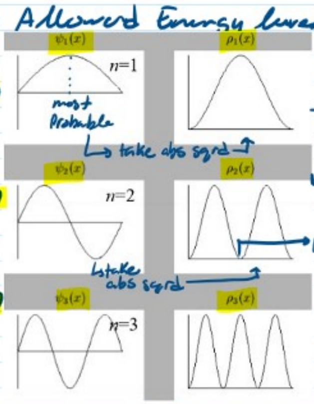
@ x=L, sin(kx)=0, kL=nπ or $n\pi = \sqrt{\frac{2mE}{\hbar^2}}L$

- Allowed Energy levels: $E(n) = \frac{n^2\pi^2\hbar^2}{2mL^2}$ → $KE = \frac{\hbar^2k^2}{2m}$

1D

2D

3D



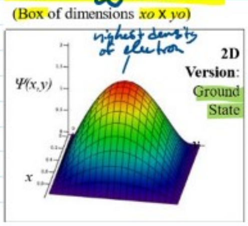
has 4x energy of 1st state

prob=0

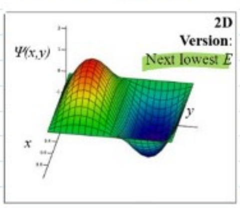
2D Box:

1st Energy level

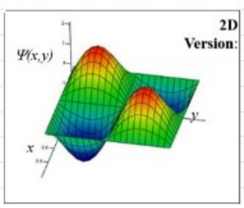
(Box of dimensions x_0 x y_0)

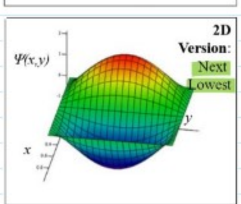


2nd Energy level



4th Energy level





1D: $E(n) = \frac{n^2\pi^2\hbar^2}{2mL}$ 2D: $E(n_x, n_y) = \frac{h^2}{8m}\left(\frac{n_x^2}{x_0^2} + \frac{n_y^2}{y_0^2}\right)$

3D: $E(n) = \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2)$