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QUANTUM CONFINEMENT

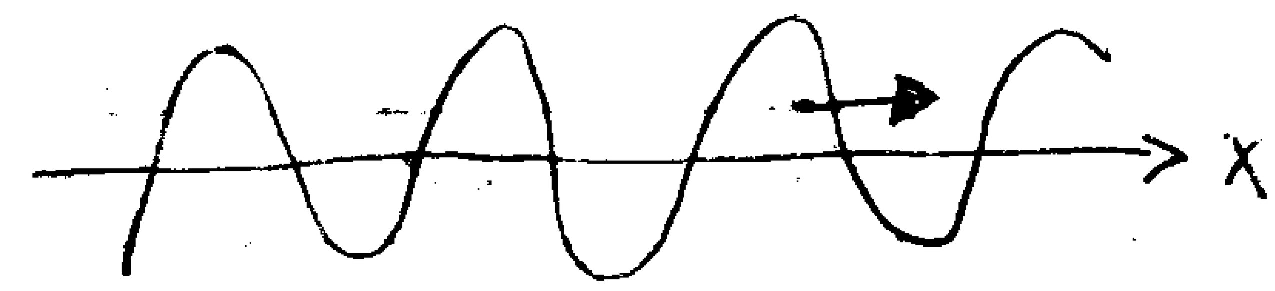
SEE Poole Ch. 9

Schrodinger wave Equation (1D)

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

$$\frac{h}{2\pi} = \hbar = 6.58\,E^{-16}\ \text{eV}\cdot\text{sec}$$

- Describes particle (e.g. electron) motion (states) along X-axis



- Quantum mechanics asserts that particle has wave-like characteristics → ONLY PROBABILITY OF BEING AT (x,t)

$$P(x,t) = |\Psi|^2 = \Psi^*(x,t)\,\Psi(x,t)$$

$$\int_{-\infty}^{\infty} \Psi^*(x)\,\Psi(x)\,\partial x = 1 \qquad \text{NORMALIZATION}$$

- Quantum mechanical operators

$$\hat{p} = i\hbar\frac{\partial}{\partial x} : \quad \langle p\rangle = \int_{-\infty}^{\infty}\Psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi^*(x,t)\,\partial x$$

Obtain expectation value of momentum

$$\hat{x} = i\hbar\frac{\partial}{\partial p} :$$

Obtain expectation value of position

$$i\hbar\frac{\partial \Psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t) = \left[\underbrace{\frac{\hat{p}^2}{2m}}_{\text{KINETIC ENERGY}} + \underbrace{V(x)}_{\text{POTENTIAL ENERGY}}\right]\Psi(x,t)$$

$$i\hbar\frac{\partial \Psi(x,t)}{\partial t} = \underbrace{\hat{H}}_{\text{HAMILTONIAN}}\Psi(x,t)$$

SEPARATION OF VARIABLES

(Similar to plane waves)

$$\Psi(x,t) = \phi(x)T(t) \longrightarrow i\hbar\frac{\partial T}{\partial t} = \underset{\text{constant}}{E}\,T(t) \rightarrow T(t) = C\exp\left(-\frac{iEt}{\hbar}\right)$$

$$\longrightarrow \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\phi(x) = E\phi(x)$$

- Solution to eigenvalue equation → specific energies E

$$\hat{H}\,\phi(x) = \underset{\text{EIGENVALUES = ENERGIES}}{E}\,\phi(x)$$

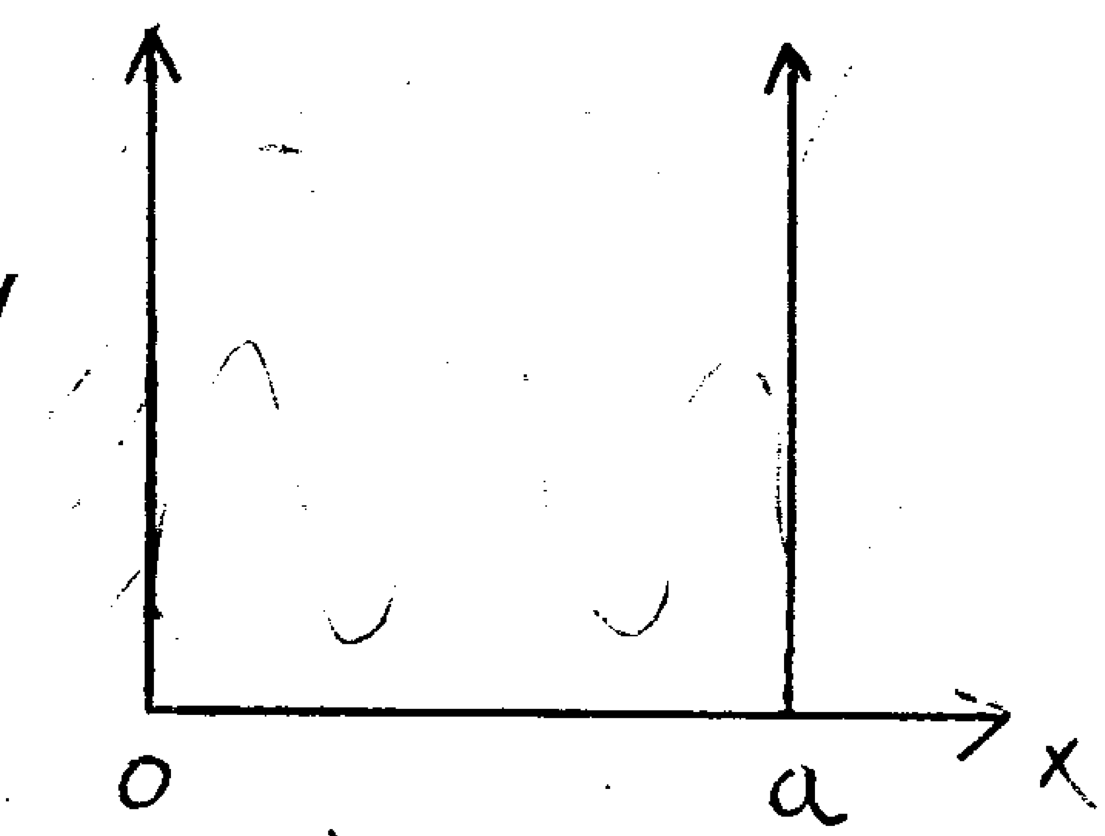
$$\psi(x,t) = \phi(x)\exp\left(-\frac{iEt}{\hbar}\right)$$

time dependent part.

Spatial part
- This is what we typically find solutions for

Particle-in-a-box

- Particle moves along x-axis, but infinite potential at 0, a



$$V = \begin{cases} \infty & (x \le 0) \\ 0 & (0 < x < a) \\ \infty & (x \ge a) \end{cases}$$

$\phi(0) = 0$, $\phi(a) = 0$ - Boundary conditions

- SOLVE EIGENVALUE EQUATION FOR $\phi(x)$ INSIDE BOX:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \cancel{V(x)}^{\,0}\right]\phi(x) = E\phi(x)$$

$$\frac{\partial^2}{\partial x^2}\phi(x) = \frac{2mE}{\hbar^2}\phi(x) = k^2\phi(x) \qquad \left(E = \frac{\hbar^2 k^2}{2m}\right)$$

General solution will be: $\phi(x) = A\exp(ikx) + B\exp(-ikx)$

FORWARD WAVE BACKWARD WAVE

BC1 $\phi(0) = 0 = A\exp(0) + B\exp(0) \rightarrow A = -B$

$$\phi(x) = 2Ai\sin(kx)$$

BC2 $\phi(a) = 0 \rightarrow ka = n\pi$, $(n = 1, 2, \ldots \infty)$

$K_n = \frac{n\pi}{a}$ [wavenumber is quantized] $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ (energy is quantized)

$\phi_n(x) = 2Ai\sin\left(\frac{n\pi x}{a}\right)$, $\int_0^a |\phi_n(x)|^2 \partial x = 1$ Normalization

$$\boxed{\phi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)} \qquad \boxed{T(t) = \exp\left(-\frac{iE_n t}{\hbar}\right)}$$

$$P_n(x,t) = |\psi_n(x,t)|^2 = \boxed{\frac{2}{a}\sin^2\left(\frac{n\pi x}{a}\right)}$$

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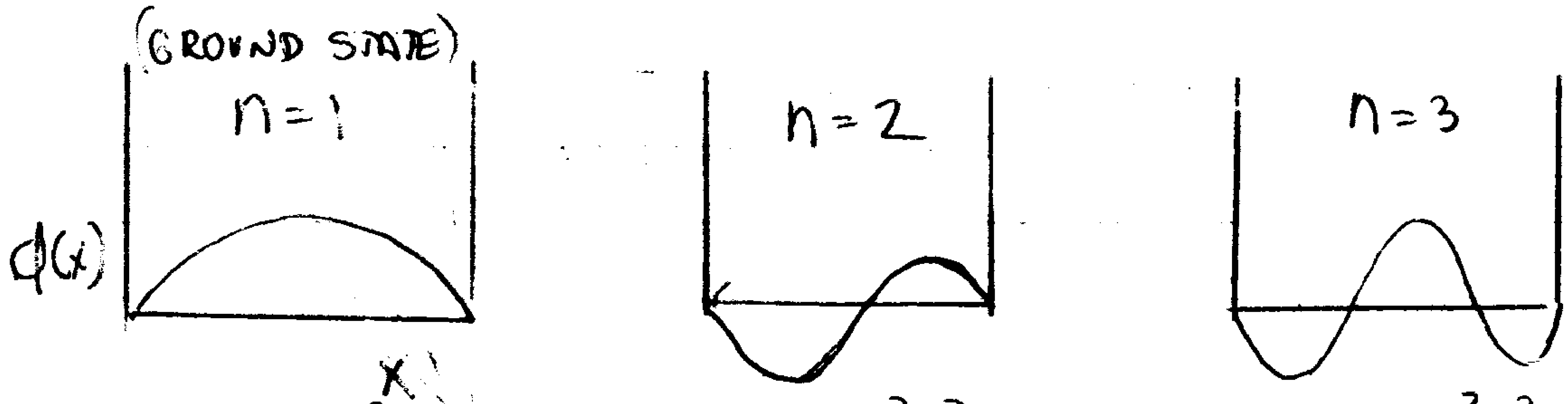


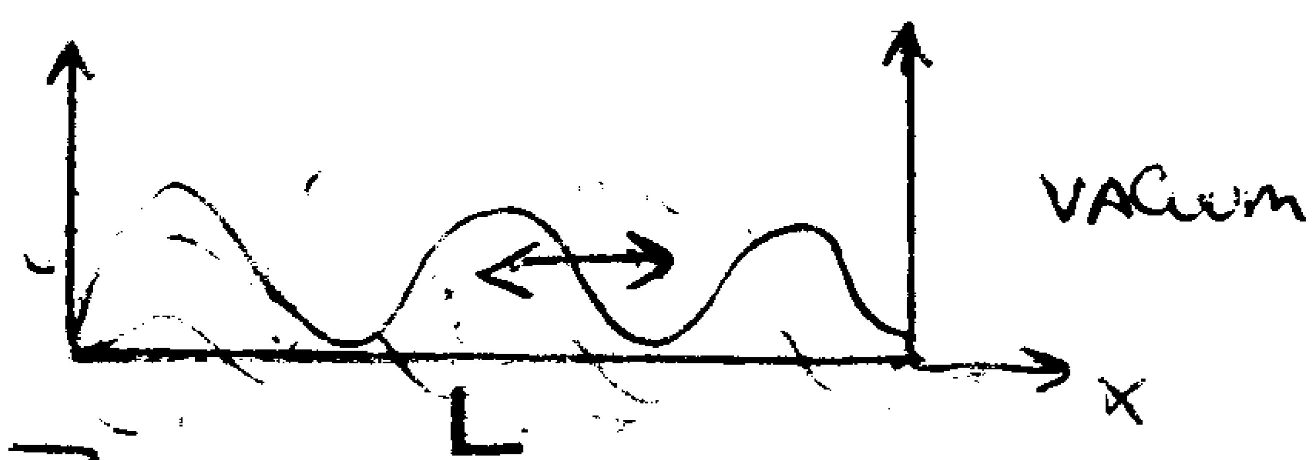
$$E_1 = \frac{\pi^2\hbar^2}{2ma^2} \qquad E_2 = \frac{2\pi^2\hbar^2}{ma^2} \qquad E_3 = \frac{9\pi^2\hbar^2}{2ma^2}$$

- "Particle" has probability function corresponding to stationary (standing) waves
- Energy can only take certain values
- SUPERPOSITION IS POSSIBLE $\Psi(x,t) = \frac{1}{\sqrt{2}}\left[\Psi_i(x,t) + \Psi_j(x,t)\right]$
  - is oscillatory behavior between states
    $\nu = \frac{E_i - E_j}{h}$ (BOHR FREQUENCY)
- UNCERTAINTY PRINCIPLE → Don't know exactly where particle is $P_1(x)$
  → $E_1 > 0$

SEE POOLE APPENDIX A.

(SOMMERFELD THEORY)

ELECTRONS IN A SOLID



- Conduction electrons CONSTRAINED TO MOVE INSIDE MATERIAL

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\Psi(x,t) \quad (3D)$$

- IN MACRO-SIZED MATERIAL, size is large (delocalization)

- BORN-VON-KARMAN Periodic Boundary conditions
  - allows wave propagation $\Psi(x) = \Psi(x+L)$

$$\phi(x) = A\exp(ikx) + B\exp(-ikx) \rightarrow \exp(ikL) = 1$$

gives: $k = \frac{2\pi n}{L}$; $E_n = \frac{\hbar^2 k^2}{2m} = \frac{2\pi^2 \hbar^2 n^2}{mL^2}$

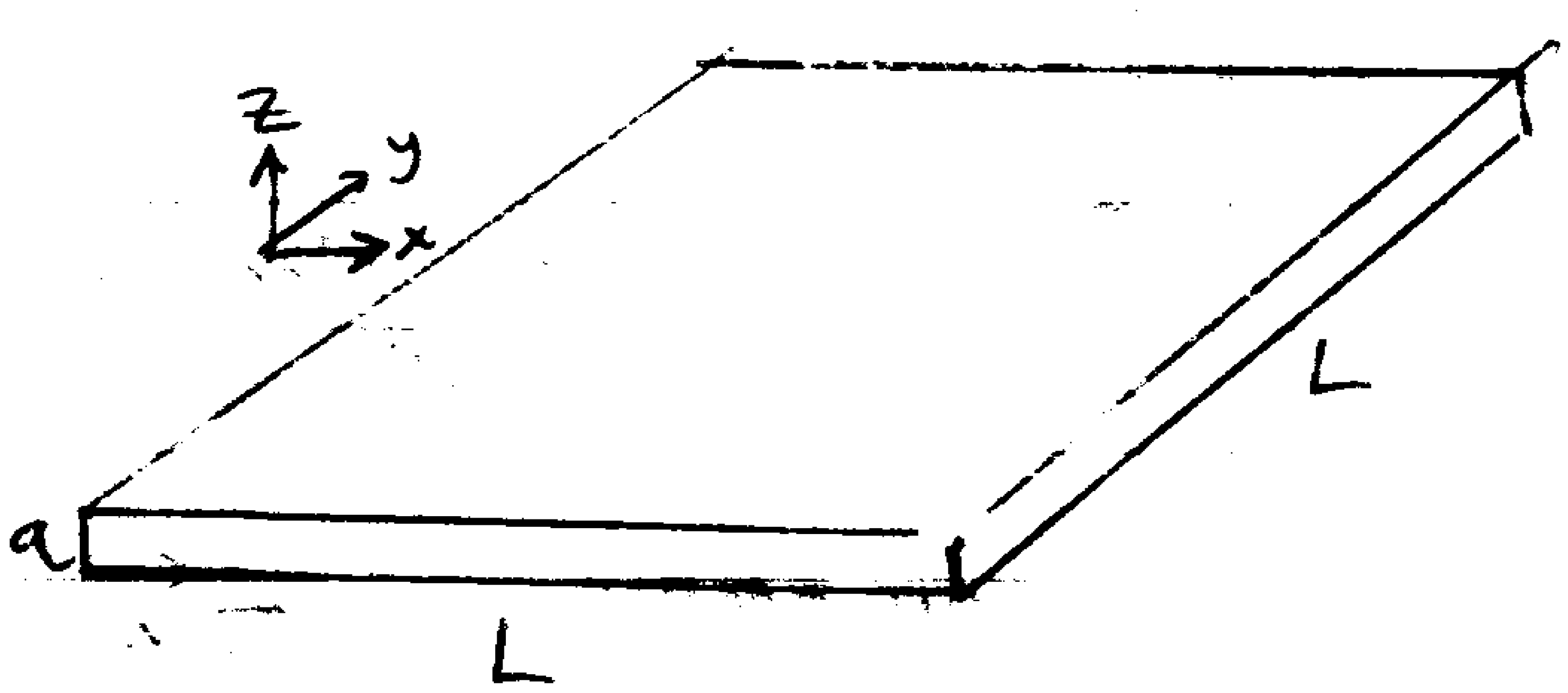
wave number

$n = 0, \pm 1, \pm 2, \ldots$ SPATIAL QUANTUM NUMBER

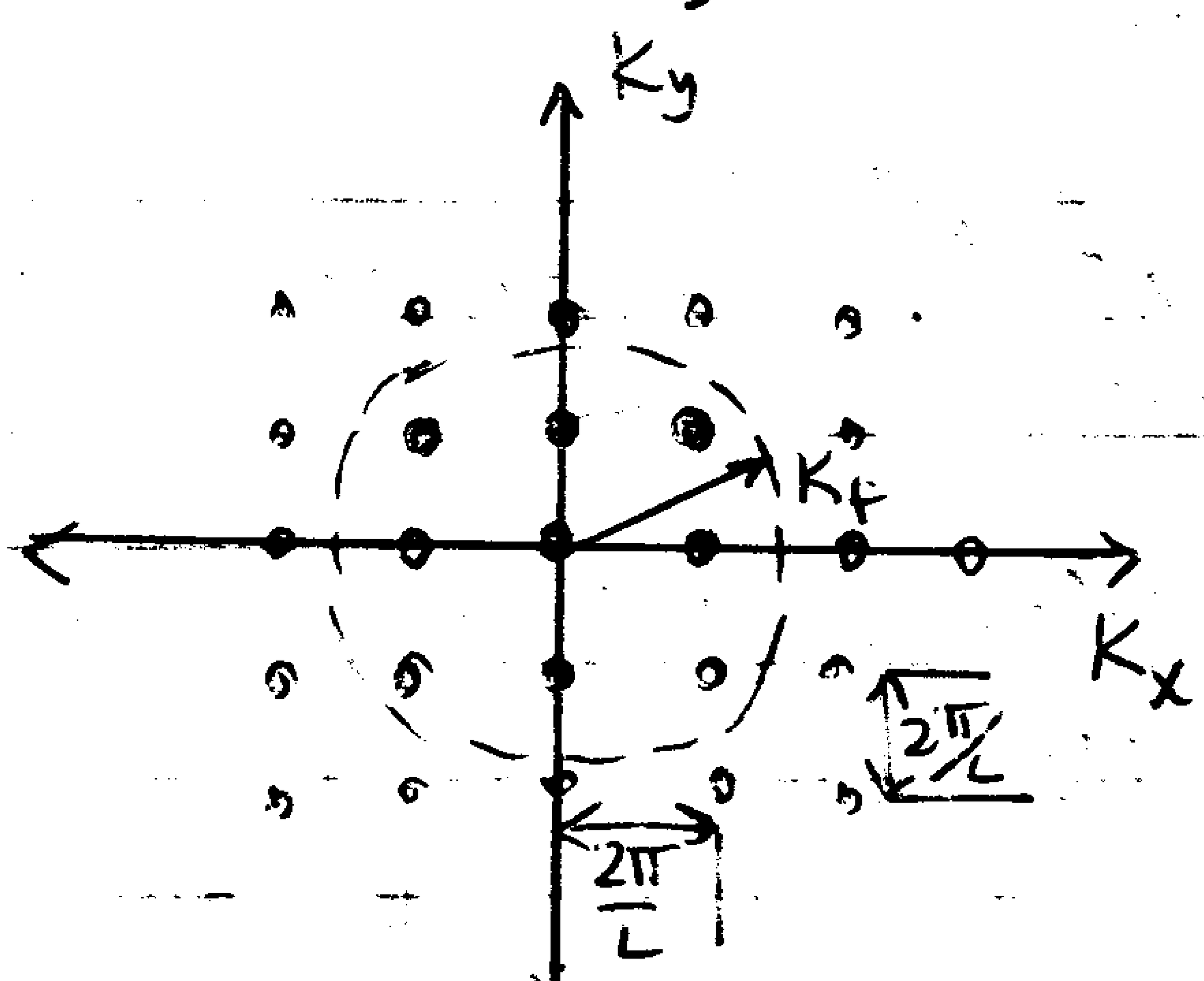
$$\varphi_n(x) = \frac{1}{\sqrt{L}} \exp\left(\frac{i 2\pi n x}{L}\right)$$ RUNNING WAVE

$$P(x) = |\varphi(x)|^2 = \frac{1}{L}$$ CONSTANT PROBABILITY EVERYWHERE IN X

II THIN FILM



- IN THE PLANE OF THE FILM, ELECRONS CAN PROPAGATE BY BVK MODEL (delocalized)



- 2 quantum numbers n_x, n_y for delocalized states '2D-ELECTRON GAS'

$$k^2 = k_x^2 + k_y^2$$

$$E = E_x + E_y$$

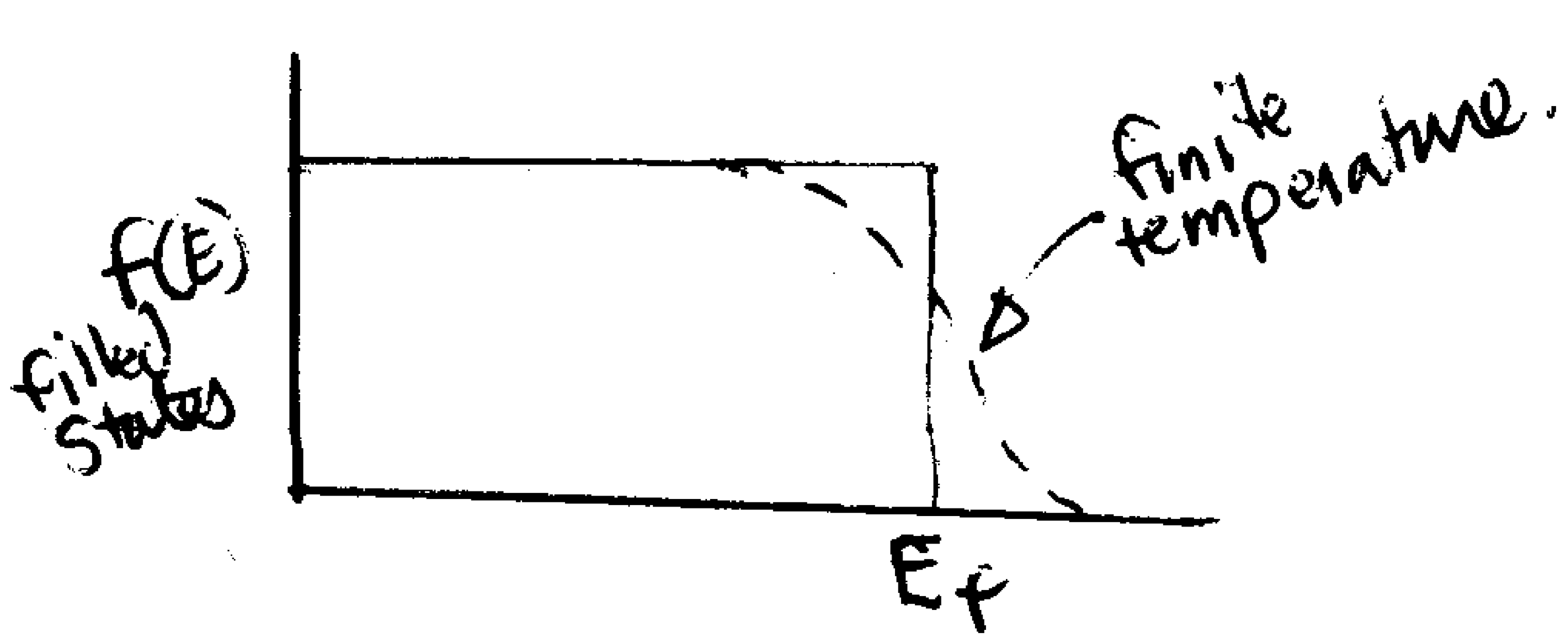
- Electrons fill available states beginning at origin (2 each ↑↓) out to k_f

$$k_f = \frac{\sqrt{2mE_f}}{\hbar}; \quad N(E) = 2 \cdot \frac{\pi k_f^2}{\left(\frac{2\pi}{L}\right)^2} = \frac{k_f^2 L^2}{2\pi} = \boxed{\frac{mL^2 E}{\pi \hbar^2}}$$

# of electron states filled

$$D(E) = \frac{\partial N(E)}{\partial E} = \frac{d}{dE}\left(\frac{mL^2 E}{\pi\hbar^2}\right) = \frac{mL^2}{\pi\hbar^2} = \text{(constant in 2D)}$$

density of states



- As L increases, spacing between states is finer, more electrons available too (in a metal)

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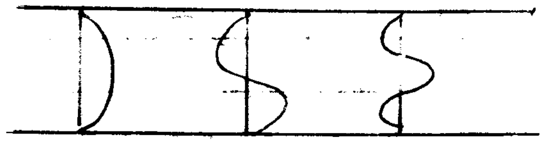
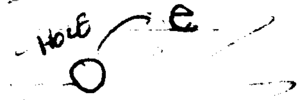
Z-direction



- Very thin so electron feels effect of boundaries
- Exists in a confined state quantized energies $E_{n_z} = \frac{\pi^2 \hbar^2}{2ma^2} n_z^2$

■ How Thin is Thin ??

(See Poole Ch. 9)



① Exciton: form electron-hole pair in solid.

~~Mott~~ Wannier Exciton

COULOMBIC POTENTIAL $F = -\frac{\overset{\text{const}}{\alpha} e^2}{\underset{\text{dielectric constant}}{\varepsilon} r^2}$

- Has solutions Like hydrogen atom
- radius $a_{eff} = \frac{0.529 \left(\frac{\varepsilon}{\varepsilon_0}\right)}{\left(\frac{m^*}{m_0}\right)} \simeq \boxed{10.4 \text{ nm in GaAs}}$

② Mean free path in metals (Weidemann-Franz)

$K_{THERM} = \frac{\ell \, V_{th} \, C_v}{3} \left(\frac{N}{V}\right)$ — electron density

ℓ — mean free path; V_{th} — Thermal velocity; C_v — heat capacity

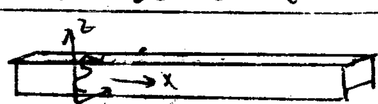
$\frac{K}{\sigma} = \frac{3}{2}\left(\frac{k_0}{e}\right)^2 T$

$\ell = \underset{\text{fermi velocity}}{V_f} \, \underset{\text{scattering time}}{\tau} = 1.5E^6 \frac{m}{sec} \cdot 3E^{-14} sec = \boxed{45 nm \text{ in Cu}}$

③ Interface states, skin depth, etc.

depends on system.

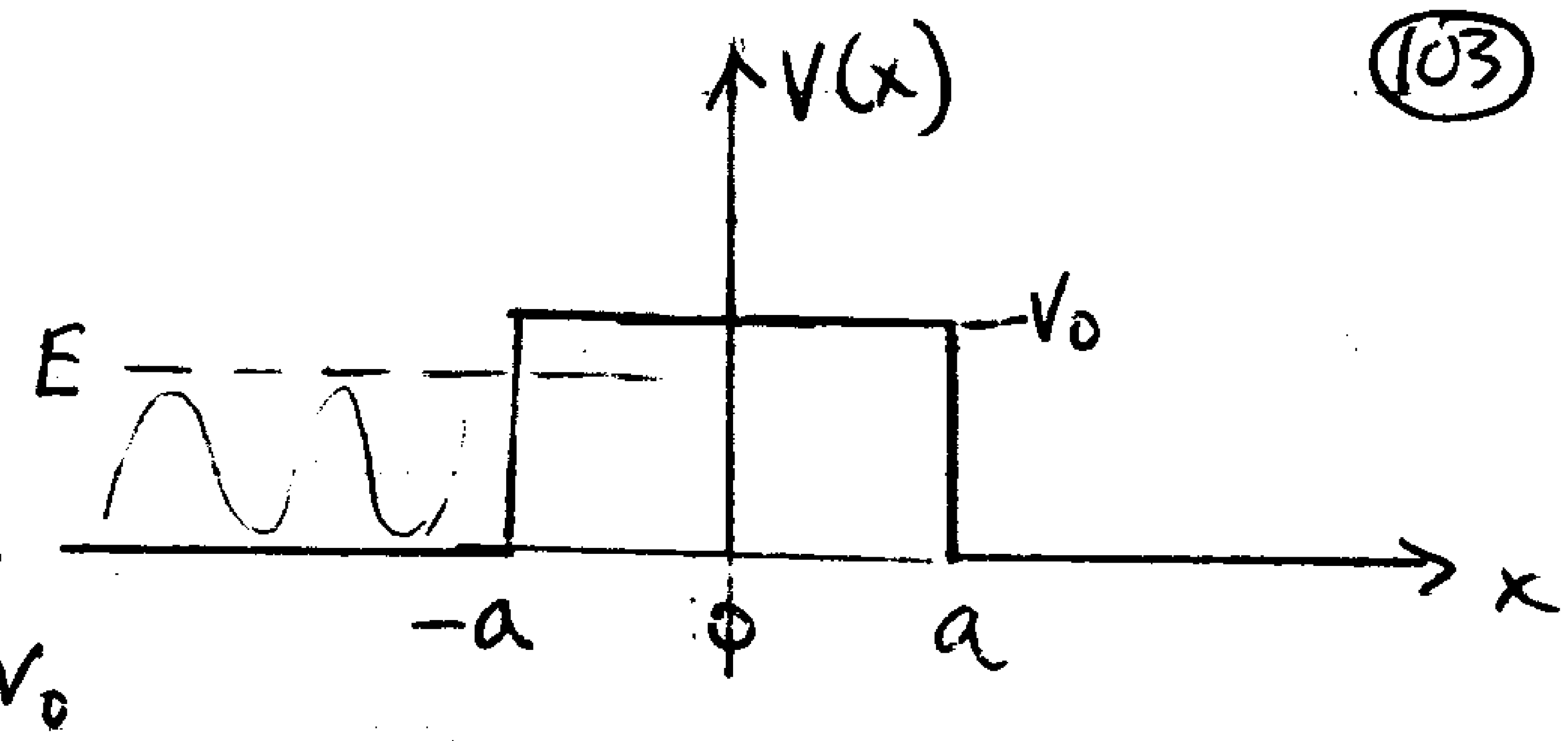
NANOWIRES & QUANTUM DOTS



WIRE: 1D - delocalized in X
- bound in y, z

DOT: 0D - bound in x, y, z
- Electron in 3D box.

QUANTUM TUNNELING.



- Electron propagation from $X = -\infty$ is INTERRUPTED BY BARRIER $0 < E < V_0$

- INSIDE BARRIER
$$-\frac{\hbar^2}{2m}\frac{\partial^2 \phi(x)}{\partial x^2} + V_0 \phi(x) = E\phi(x)$$

$$\frac{\partial^2 \phi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\phi(x) = 0$$

- SOLUTION $\alpha = \frac{2m(V_0 - E)}{\hbar^2}$

$$\phi(x) = Ae^{+\alpha x} + Be^{-\alpha x} \qquad |x| < a \text{ inside barrier}$$

$$\phi(x) = e^{ikx} + Re^{-ikx} \qquad x < -a \text{ incident + reflected.}$$

$$\phi(x) = Te^{ikx} \qquad x > a \text{ Transmitted}$$

- Apply boundary conditions at $\pm a$ see Goswami Ch. 4

$$|T|^2 = \frac{(2k\alpha)^2}{(k^2+\alpha^2)^2 \sinh^2(2\alpha a) + (2k\alpha)^2} \sim e^{-4\alpha a}$$

- Finite probability for particle to tunnel through barrier