

STEFANO
CURTAROW

SOME SCHRÖDINGER SOLUTIONS

- INFINITE WELL
- FINITE WELL
- TRANSMISSION / REFLECTION
- POTENTIAL STEP
- THEORY OF MEASURE (why here?)

$$Q_{MA1} - Q_{MA9} + \text{EXTRA}$$

SOMMERFELD THEORY ELECTRON GAS

CHAP 2 AM.

Free electrons in a box

STATIONARY SCHRÖDINGER EQUATION (TIME INVARIANT (stationary))

$$\hat{H}\psi = E\psi \Rightarrow \text{defines } \psi$$

real solutions are

eigen-vectors $(\psi(x))_n$

of Hamiltonian generator (Energy)

with $E_{\text{energi}}(n)$

ψ is wave function

$$\int \psi^* \psi dx = 1$$

$$|\psi(x)|^2 dx^3 = \psi^* \psi dx^3 = \text{prob to find electron in } [x, x+dx]$$

Volume of dx^3

Other properties are operators

$$\hat{O} = \langle \hat{O} \rangle \equiv \int \psi^*(x) \hat{O} \psi(x) dx = \sum (\psi^*) (\hat{O}) (\psi)$$

↑ ↑
operator average of an operator over the density

$$\text{but this is Real} \Rightarrow \hat{O}^\dagger = \hat{O} \Rightarrow \hat{O} = \hat{O}^\dagger$$

self adjoint

adjoint for matrices
would be -complex conjugate
-transpose

$\hat{H}$ = Energy operator $\Rightarrow$

Hamiltonian $\hat{T} + \hat{V}$

$$\frac{\hat{p}^2}{2m} + V = -\frac{\hbar^2}{2m} \left(\frac{\partial}{\partial x} \right)^2 + V(x) = \hat{H}(x)$$

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

$\hat{p} = \hbar k$

$\hbar k = -i\hbar \left(\frac{\partial}{\partial x} = +ik \right) = \hbar k$

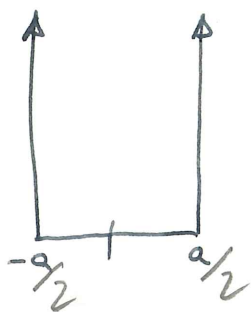
DE BROGLIE says

POSTULATE

$$\lambda = \frac{h}{p} \quad k = \frac{2\pi}{\lambda}$$

$$p = \frac{h}{\lambda} = \frac{h k}{2\pi} \Rightarrow p = \hbar k$$

SOLUTION EQ SCHRÖDINGER



$$V(x) = \begin{cases} 0 & |x| \leq a/2 \\ +\infty & |x| \geq a/2 \end{cases}$$

INFINITE WELL

CLASSICAL

$$P(x) \approx \text{constant} \Rightarrow \frac{1}{a}$$

$$\langle x \rangle_a = 0$$

$$\langle x^2 \rangle = \frac{a^2}{12}$$

QM.

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] \psi(x,t) = -i\hbar \frac{\partial}{\partial t} \psi(x,t)$$

STATIONARY

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

INSIDE THE WELL

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

$$\psi = e^{ikx}$$

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

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

$$\Rightarrow k = \pm \sqrt{\dots}, \pm k$$

$$\psi = a e^{ikx} + b e^{-ikx} =$$

$$= A \sin(kx) + B \cos(kx)$$

$$V(\text{outside}) = \infty$$

$$\psi \Rightarrow 0$$

$$\psi(-a/2) = \psi(a/2) = 0$$

$$\left. \begin{aligned} -A \sin\left(\frac{ka}{2}\right) + B \cos\left(\frac{ka}{2}\right) &= 0 \\ A \sin\left(\frac{ka}{2}\right) + B \cos\left(\frac{ka}{2}\right) &= 0 \end{aligned} \right\} \begin{aligned} \rightarrow 2B \cos\left(\frac{ka}{2}\right) &= 0, A=0 \\ \rightarrow 2A \sin\left(\frac{ka}{2}\right) &= 0, B=0 \end{aligned}$$

QMA1

Solution $A=0$

$$\cos\left(\frac{ka}{2}\right) = 0 \Rightarrow$$

$$\psi = B \cos(km x)$$

SYMMETRIC

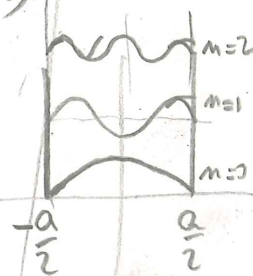
$$\Rightarrow \frac{\pi}{2} + n\pi = \frac{\pi}{2}(2m+1) \Rightarrow km$$

$$\Rightarrow \frac{ka}{2} = \frac{\pi}{2}(2m+1) \Rightarrow k_m = \frac{\pi}{a}(2m+1)$$

$$\Rightarrow \frac{2m E_m}{\hbar^2} = \left[\frac{\pi}{a}(2m+1) \right]^2$$

$$E_m = \frac{\hbar^2}{2m} \left[\frac{\pi}{a}(2m+1) \right]^2$$

1, 3, 5, 7



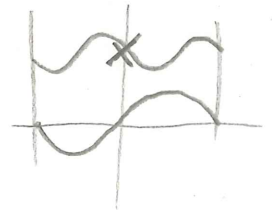
Solution $B=0$

$$\sin\left(\frac{ka}{2}\right) = 0$$

$$\frac{ka}{2} = n\pi \Rightarrow$$

$$\psi = A \sin(kx)$$

$$k_m = \frac{\pi}{2a} 2m$$



$$\Rightarrow \frac{2m E_m}{\hbar^2} = \left[\frac{\pi}{a}(2m) \right]^2 \Rightarrow E_m = \frac{\hbar^2}{2m} \left[\frac{\pi}{a}(2m) \right]^2$$

2, 4, 6, ...

$$E_n = \frac{\hbar^2}{2m} \left[\frac{n\pi}{a} \right]^2 \begin{cases} n = \text{ODD} \Rightarrow \psi \propto \cos(k_m x) \\ n = \text{EVEN} \Rightarrow \psi \propto \sin(k_m x) \end{cases} \quad k_m = \frac{\pi}{a} n$$

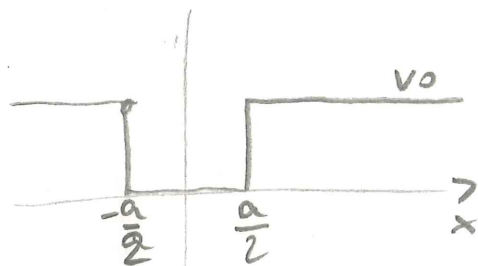
$$\psi_m = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right)$$

$$\psi_m = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

QMA2.

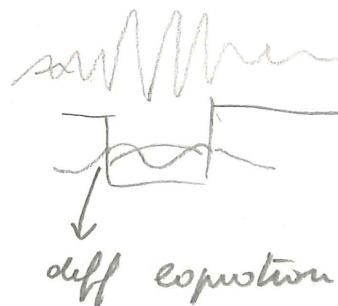
FINITE WELL

$$V(x) = \begin{cases} 0 & |x| \leq a/2 \\ V_0 & |x| \geq a/2 \end{cases}$$



$$E > V_0$$

$$E < V_0$$



⇒ SOLUTION is $C_1(x)$
continuous and $\frac{d}{dx}$ continuous

$$E \leq V_0 \begin{cases} \text{inside} & -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi = E \psi \\ \text{outside} & -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi = (E - V_0) \psi \end{cases}$$

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

depending on $(E - V_0) \geq 0$
different solutions

$E < V_0$ BOUNDED STATE

inside $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi = E \psi \quad \sim \quad \psi = A \sin(kx) + B \cos(kx)$

outside $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi = \underbrace{(E - V_0)}_{< 0} \psi \Rightarrow \psi = A_1 e^{-\eta x} + B_1 e^{\eta x}$

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

↓ picks the positive

CONTINUITY

$$x \leq -\frac{a}{2}$$

$$\psi = B_1 e^{\eta x}$$

$$-\frac{a}{2} \leq x \leq \frac{a}{2}$$

$$\psi = A \sin(kx) + B \cos(kx)$$

$$x \geq \frac{a}{2}$$

$$\psi = A_1 e^{-\eta x}$$

ANTI EVEN
ODD SOLUTION
EVEN SOLUTION
ODD SYM
 $B_1 = -A_1$
 $A_1 = B_1$

~~EVEN~~ ^{SIMMETRIC} $A=0$
continuity

$$\Rightarrow \left\{ \begin{array}{l} C e^{\eta x} \\ B \cos(kx) \\ C e^{-\eta x} \end{array} \right\}$$

$$\text{ODD} \left\{ \begin{array}{l} -C \\ B \sin \\ = C \end{array} \right.$$

$$1) B \cos\left(\frac{\kappa a}{2}\right) = C e^{-\eta a/2}$$

derivative

$$2) -B \kappa \sin\left(\frac{\kappa a}{2}\right) = -\eta C e^{-\eta a/2}$$

$$\frac{2 \cos}{2 \sin} = -\sin$$

ratio

$$\frac{-B \kappa \sin(C)}{B \cos(C)} = \frac{-\eta C e^{-\eta a/2}}{C e^{-\eta a/2}}$$

$$\kappa \tan\left(\frac{\kappa a}{2}\right) = \eta$$

~~EVEN~~ ^{SYM} $\kappa \tan(\kappa a/2) = \eta$

~~ODD~~ ^{ANTI} $-\kappa \cot(\kappa a/2) = \eta$

$$y = \frac{\kappa a}{2}$$

$$R = \sqrt{\frac{2m V_0}{\hbar^2} \left(\frac{a}{2}\right)^2}$$

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

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

$\rightarrow -\kappa^2$

$$\Rightarrow \frac{\kappa a}{2} \tan\left(\frac{\kappa a}{2}\right) = \frac{\eta a}{2}$$

$\downarrow$ y $\downarrow$ y $\downarrow$ y

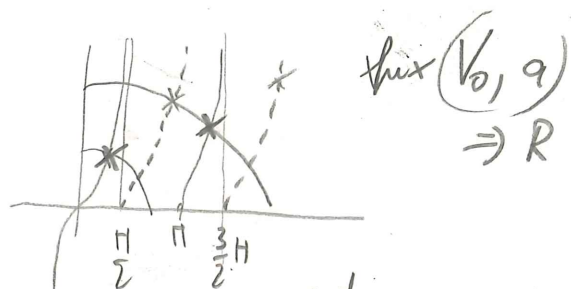
$$y \tan y = \sqrt{R^2 - y^2}$$

circle radius R

$$-y \cot y = \sqrt{R^2 - y^2}$$

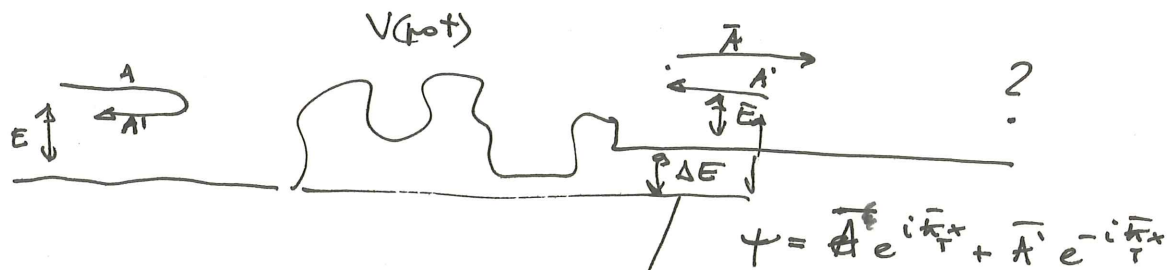
$$\eta^2 \left(\frac{a}{2}\right)^2 = \frac{2m V_0}{\hbar^2} \left(\frac{a}{2}\right)^2 - \underbrace{\kappa^2 \left(\frac{a}{2}\right)^2}_{y^2}$$

R^2 y^2



get $y_n \Rightarrow \underline{\underline{\kappa_n}}$

TRANSMISSION MATRIX



$$\psi = A e^{i k x} + A' e^{-i k x}$$

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

$$\hbar \Delta E = 0 \Rightarrow \kappa =$$

$$\bar{\kappa} = \sqrt{\frac{2m(E - \Delta E)}{\hbar^2}}$$

$$\begin{aligned} \bar{A} &= F(\kappa) A + F'(\kappa) A' \\ \bar{A}' &= G(\kappa) A + G'(\kappa) A' \end{aligned}$$

$$\Rightarrow M(\kappa) = \begin{pmatrix} F(\kappa) & F'(\kappa) \\ G(\kappa) & G'(\kappa) \end{pmatrix}$$

$$\begin{pmatrix} \bar{A} \\ \bar{A}' \end{pmatrix} = M(\kappa) \begin{pmatrix} A \\ A' \end{pmatrix} \quad \text{TRANSMISSION MATRIX}$$

$$R_{\text{reflection}}(\kappa) \equiv \left| \frac{A'(\kappa)}{A(\kappa)} \right|^2 = \left| \frac{G}{F} \right|^2$$

$$T_{\text{transmission}}(\kappa) \equiv \left| \frac{\bar{A}(\kappa)}{A(\kappa)} \right|^2 = \frac{1}{|F(\kappa)|^2} \quad \text{if } \bar{A}' = 0$$

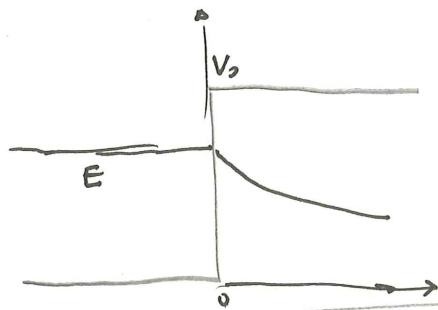
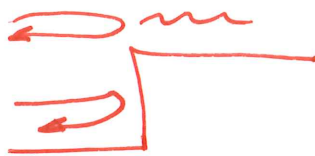
$$R + T = 1$$

conservation of probability

if $\Delta E = 0$, symmetrical or not

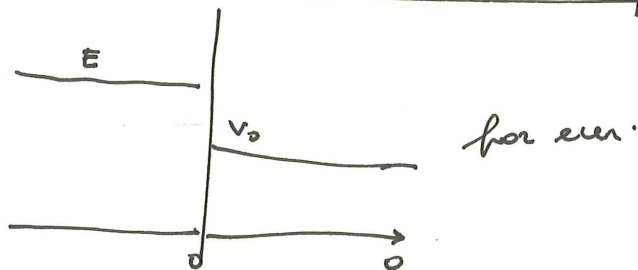
$$\Rightarrow R, T \text{ from Right} \Leftrightarrow T, R \text{ from left}$$

POTENTIAL STEP



$$E < V_0 \Rightarrow T = 0 \Rightarrow R = 1$$

RAGE LEFT TO RIGHT INCIDENT



$$\psi_i = A e^{i k_i x} + A' e^{-i k_i x} \quad x < 0$$

$$\psi_T = \bar{A} e^{i k_T x} + 0 \quad \text{nothing at right}$$

$$k_i = \sqrt{\frac{2mE}{\hbar^2}} \sim \sqrt{E}$$

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

$$k_T^2 = k_i^2 - \frac{2mV_0}{\hbar^2}$$

$$\psi(0) = A + A' = \bar{A} \quad \text{continuity}$$

$$\psi'(0) = i k_i A - i k_i A' = i k_T \bar{A}$$

$$\Rightarrow k_i (A - A') = k_T \bar{A} \Rightarrow \frac{A - A'}{A + A'}$$

$$\Rightarrow k_i (A - A') = k_T (A + A') \Rightarrow \frac{A - A'}{A + A'}$$

$$A (k_i - k_T) = A' (k_T + k_i)$$

$$\Rightarrow \frac{A'}{A} = \frac{k_i - k_T}{k_i + k_T}$$

$$R = \left| \frac{A'}{A} \right|^2$$

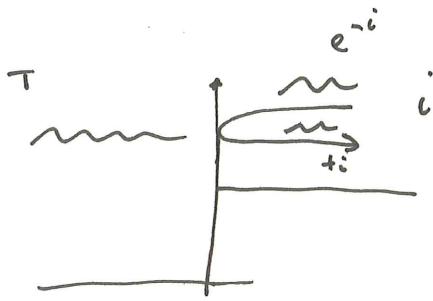
$$T = \left| \frac{\bar{A}}{A} \right|^2$$

CLASSIC
 $R = 0$
 $T = 1$
 $E \gg V_0$

$$R = \left(\frac{\sqrt{E} - \sqrt{E-V_0}}{\sqrt{E} + \sqrt{E-V_0}} \right)^2$$

$$\Rightarrow T = 1 - R$$

RIGHT TO LEFT



$$\psi_i = A e^{-i k_T x} + A' e^{i k_i x}$$

$$\psi_T = \bar{A} e^{-i k_T x}$$

$$\psi(0) = A + A' = \bar{A}$$

$$\psi'(0) = -i k_i A + A' i k_i = -i k_T \bar{A}$$

$\downarrow$
 $A + A'$

$$\downarrow$$

$$k_i (A' - A) = -k_T (A + A')$$

$$\Rightarrow k_T (A + A') = k_i (A - A')$$

$$A' (k_T + k_i) = A (k_i - k_T)$$

$$\Rightarrow R = \left| \frac{k_i - k_T}{k_T + k_i} \right|^2 = \left| \frac{\sqrt{E} - \sqrt{E + V_0}}{\sqrt{E} + \sqrt{E + V_0}} \right|^2 \Rightarrow T = 1 - R \text{ etc}$$

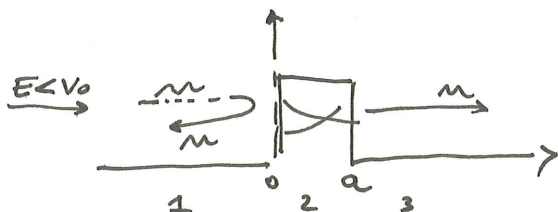
$$R = \left| \frac{A'}{A} \right|^2$$

$$T = 1 - R$$

$$k_i \sim \sqrt{E - V_0}$$

$$k_T \sim \sqrt{E}$$

POTENTIAL WELL $V_0 > 0$ $E < V_0$ classic $R=1$ $T=0$



$$k_1 = k_3 = \sqrt{\frac{2mE}{\hbar^2}}$$

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

$$\psi_1 = A e^{ikx} + A' e^{-ikx}$$

$$\psi_2 = B e^{\eta x} + B' e^{-\eta x}$$

$$\psi_3 = \bar{A} e^{ikx}$$

$$\psi(0) = A + A' = B + B' \Rightarrow B' = A + A' - B$$

$$\psi'(0) = ikA - ikA' = \eta B - \eta B' \Rightarrow ik(A - A') = \eta(B - B')$$

$$\psi(a) = B e^{\eta a} + B' e^{-\eta a} = \bar{A} e^{ika} \Rightarrow \bar{A} = \frac{B e^{\eta a} + B' e^{-\eta a}}{e^{ika}}$$

$$\psi'(a) = \eta B e^{\eta a} - \eta B' e^{-\eta a} = \bar{A} i k e^{ika}$$

$$\bar{A} = \frac{\eta(B e^{\eta a} - B' e^{-\eta a})}{i k e^{ika}}$$

$$ik(A - A') = \eta(B - A - A' + B) = \eta(2B - A - A')$$

$$\eta, k \in \mathbb{R}$$

$$ik(A - A') + \eta(A + A') = 2B\eta$$

$$B = \frac{ik(A - A') + \eta(A + A')}{2\eta}$$

$$B' = \frac{-ik(A - A') + \eta(A + A')}{2\eta}$$

$$\bar{A} = \frac{B e^{\eta a} + B' e^{-\eta a}}{e^{ika}} = \frac{\eta(B e^{\eta a} - B' e^{-\eta a})}{i k e^{ika}}$$

$\Rightarrow$ $\bar{A}$

Q.M.A.B

$$\Rightarrow ik(A-A')e^{\eta a} + \eta(A+A')e^{\eta a} - ik(A-A')e^{-\eta a} + \eta(A+A')e^{-\eta a} =$$

$$= \cancel{\frac{\eta}{ik}} \eta(A-A')e^{\eta a} + \frac{\eta^2}{ik}(A+A')e^{\eta a} + \eta(A-A')e^{-\eta a} - \frac{\eta^2}{ik}(A+A')e^{-\eta a}$$

solve $\Rightarrow$

$$A(ike^{\eta a} + \cancel{\eta e^{\eta a}} - ik e^{-\eta a} + \cancel{\eta e^{-\eta a}} - \cancel{\eta e^{\eta a}} - \frac{\eta^2}{ik} e^{\eta a} - \cancel{\eta e^{-\eta a}} + \frac{\eta^2}{ik} e^{-\eta a}) =$$

$$A'(ike^{\eta a} - \cancel{\eta e^{\eta a}} - ik e^{-\eta a} - \cancel{\eta e^{-\eta a}} - \cancel{\eta e^{\eta a}} + \frac{\eta^2}{ik} e^{\eta a} - \cancel{\eta e^{-\eta a}} - \frac{\eta^2}{ik} e^{-\eta a})$$

$$A \left[ik(e^{\eta a} - e^{-\eta a}) - \frac{\eta^2}{ik}(e^{\eta a} - e^{-\eta a}) \right] = \frac{e^x + e^{-x}}{2} = \cosh x$$

$$\frac{e^x - e^{-x}}{2} = \sinh x$$

$$A' \left[ik(e^{\eta a} - e^{-\eta a}) - 2\eta(e^{\eta a} + e^{-\eta a}) + \frac{\eta^2}{ik}(e^{\eta a} - e^{-\eta a}) \right]$$

$$\Rightarrow A \left[2ik \sinh(\eta a) + \frac{i\eta^2}{k} \sinh(\eta a) \right]$$

$$A \left[2ik \sinh(\eta a) + \frac{i\eta^2}{k} \sinh(\eta a) \right] = A' \left[2ik \sinh \eta a - 4\eta \cosh \eta a - \frac{2i\eta^2}{k} \sinh(\eta a) \right]$$

$$\frac{A'}{A} = \frac{k \sinh + \eta^2/k \sinh}{k \sinh + 2i\eta \cosh - \eta^2/k \sinh}$$

$$= \frac{(k^2 + \eta^2) \sinh(\eta a)}{(k^2 - \eta^2) \sinh(\eta a) + 2ik\eta \cosh(\eta a)}$$

$$\cosh^2 - \sinh^2 = 1$$

$\Rightarrow$

$$R = \frac{(k^2 + \eta^2)^2 \sinh^2(\eta a)}{(k^2 - \eta^2)^2 \sinh^2(\eta a) + 4k^2 \eta^2 \cosh^2(\eta a)}$$

QMA9

$$\frac{(k^2 + \eta^2)^2 \sinh^2(\eta a)}{(k^2 - \eta^2)^2 \sinh^2(\eta a) + 4k^2 \eta^2 \cosh^2(\eta a)}$$

$$- [k^2 \eta^2 \sinh^2 - 2 \cosh^2 + 4 \cosh^2] = 1 + 2 \cosh^2$$

$$R = \frac{(k^2 + \eta^2)^2 \sinh^2(\eta a)}{(k^4 - 2\eta^2 k^2 + \eta^4) \sinh^2(\eta a) + 4k^2 \eta^2 (\cosh^2 \eta)}$$

$$\cosh^2 - \sinh^2 = 1$$

$$\cosh^2 = 1 + \sinh^2$$

$$+ \frac{4k^2 \eta^2 (\cosh^2 \eta)}{4k^2 \eta^2 + 4k^2 \eta^2 \sinh^2}$$

$$\Rightarrow R = \frac{(k^2 + \eta^2)^2 \sinh^2(\eta a)}{(k^2 + \eta^2)^2 \sinh^2(\eta a) + 4k^2 \eta^2}$$

$$T = \frac{4\eta^2 k^2}{(k^2 + \eta^2)^2 \sinh^2(\eta a) + 4k^2 \eta^2}$$

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

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

$$\text{if } \eta a \gg 1 \quad T \approx 16\delta (1-\delta) e^{-2\eta a}$$

$$E < V_0$$

$$\delta = E/V_0$$

Never 0!!

if $E > V_0$

$$T = \frac{4k^2 K^2}{(k^2 - K^2) \sin^2(Ka) + 4k^2 K^2}$$

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

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

$$R = \frac{(k^2 - K^2) \sin^2(Ka)}{(k^2 - K^2) \sin^2(Ka) + 4k^2 K^2}$$

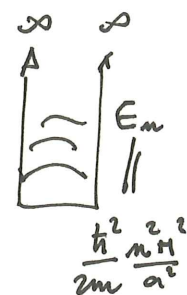
$$\sin^2(Ka) = 0 \text{ if } Ka = n\pi$$

$$Ka = n\pi \quad K^2 a^2 = n^2 \pi^2$$

$$\frac{2m(E - V_0)}{\hbar^2} a^2 = n^2 \pi^2$$

$$\Rightarrow \frac{n^2 \pi^2 \hbar^2}{2m} = (E - V_0) a^2$$

$$E = V_0 + \frac{n^2 \pi^2 \hbar^2}{2m a^2} = V_0 + E_{\text{energy}}$$



Q4A 6

THEORY OF MEASURE

have a system, & $\hat{H}\psi = E\psi \Rightarrow \psi_n$ eigen vector
 E_n eigen values.

I make a measure, I get $E_1, E_2, E_3, \dots, E_n$
 one of the eigen vectors with probability $P_1 \dots P_2 \dots P_n$

What was the state of the system?

was a general state

$$\psi \Rightarrow \hat{H}\psi = ? \quad E = ?$$

measure
 E

$$\psi = a_1\psi_1 + a_2\psi_2 + \dots = \sum_n a_n\psi_n$$

eigen vector.

$$E = \int \psi \hat{H} \psi dx =$$

$$= \sum_{ij} \int a_i^* a_j \psi_i^* \hat{H} \psi_j dx =$$

$$\Rightarrow E = \sum_{ij} a_i^* a_j E_j \int \psi_i \psi_j dx =$$

$$= \sum_n |a_n|^2 E_n$$

a_i = scalar product
 of ψ_n and ψ

$\Rightarrow$ how much ψ_n
 is inside ψ

$$a_n = \int \psi_n^* \psi dx$$

OR $\langle \psi_n | \psi \rangle$

$$\langle E \rangle_{\text{meas}} = \sum_n |a_n|^2 E_n$$

one of the outcomes

$P_n = |a_n|^2$ is probability
 of getting.

E_n as measure!