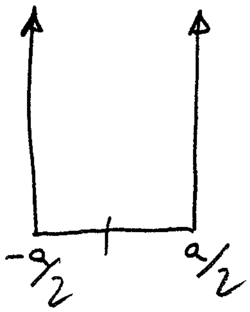
STEFANO
CURTAROLO

SOME SCHRODINGER SOLUTIONS

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

QMA1 - QMA9 + EXTRA

SOLUTION EQ SCHRODINGER



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

INFINITE WELL

CLASSICAL

$P(x) \simeq \text{constant} \doteq \frac{1}{a} \Rightarrow$ $\langle x \rangle_a = 0$

$\langle x^2 \rangle = a^2/12$

QM.

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

STATIONARY

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

INSIDE THE WELL

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

$$\cancel{\psi} \qquad \frac{+\hbar^2}{2m} + k^2 = E \qquad k = \pm \sqrt{\frac{2mE}{\hbar^2}}$$

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

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

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

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

$\psi \Rightarrow 0$

$$\psi\left(-\frac{a}{2}\right) = \psi\left(\frac{a}{2}\right) = 0$$

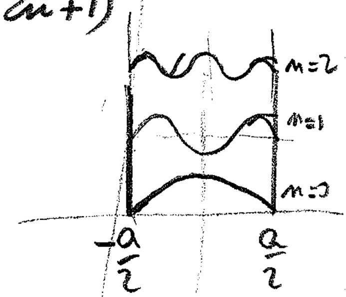
$$\left.\begin{aligned} -A \sin\left(\frac{ka}{2}\right) + B \cos\left(\frac{ka}{2}\right) &= 0 \\ A \sin\left(\frac{ka}{2}\right) + B \cos\left(\frac{ka}{2}\right) &= 0 \end{aligned}\right\} \quad \begin{aligned} &\Sigma \to 2B \cos(ka/2) = 0 \;, \cancel{A=0} \\ &- \to 2A \sin(ka/2) = 0 \;, B = 0 \end{aligned}$$

Solution $A=0$ $\quad \cos\left(\frac{ka}{2}\right)=0 \Rightarrow \quad \psi = B\cos(k_n x)$

SYMMETRIC

$\hookrightarrow \frac{\pi}{2} + n\pi = \frac{\pi}{2}(2n+1) \Rightarrow k_n$

$$\Rightarrow \frac{ka}{2} = \frac{\pi}{2}(2n+1) \Rightarrow k_n = \frac{\pi}{a}(2n+1)$$



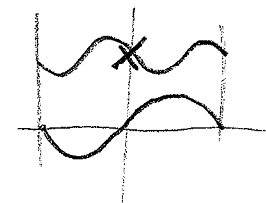
$$\Rightarrow \frac{2mE_n}{\hbar^2} = \left[\frac{\pi}{a}(2n+1)\right]^2$$

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

1, 3, 5, 7

SOLUTION $B=0$ $\quad \sin\left(\frac{ka}{2}\right)=0 \quad \frac{ka}{2} = n\pi \Rightarrow \quad \psi = A\sin(kx)$

$$k_n = \frac{\pi}{a}2n$$



$$\Rightarrow \frac{2mE_n}{\hbar^2} = \frac{\pi}{a}(2n) \Rightarrow \quad E_n = \frac{\hbar^2}{2m}\left[\frac{\pi}{a}(2n)\right]^2$$

2, 4, 6 ...

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

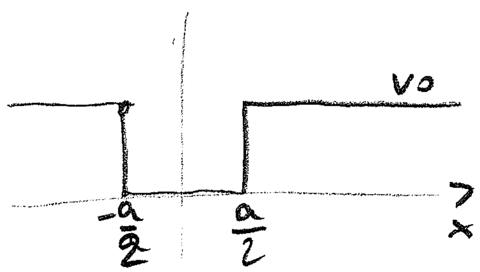
$$\psi_n = \sqrt{\frac{2}{a}}\cos\left(\frac{n\pi x}{a}\right)$$

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

QM42.

FINITE WELL

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



$E > V_0$

$E < V_0$

diff equation

$\Rightarrow$ SOLUTION is $C_1(x)$

continuous and $\frac{\partial}{\partial x}$ continuous

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

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

depending on $(E - V_0) \gtrless 0$

different solutions

$E < V_0$ BOUNDED STATE

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

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

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

pick the positive

- CONTINUITY

$x \leq -\frac{a}{2} \qquad \psi = B_1 e^{\eta x}$

$-\frac{a}{2} \leq x \leq a/2 \qquad \psi = A\sin(kx) + B\cos(kx)$

$\longrightarrow$ ODD SOLUTION $\quad B_1 = -A_1$

EVEN SOLUTION $\quad A_1 = B_1$

$x \geq a/2 \qquad \psi = A_1 e^{-\eta x}$

QMA3

EVEN $A=0$ $\Rightarrow \left\{ \begin{array}{l} Ce^{\eta x} \\ B\cos(kx) \\ Ce^{-\eta x} \end{array} \right\}$ ODD $\left| \begin{array}{l} -C \\ B\sin \\ C \end{array} \right.$

continuity

$2\cos = -\sin$

1) $B\cos\left(\frac{ka}{2}\right) = Ce^{-\eta a/2}$

derivobility

ratio

2) $-Bk\sin\left(\frac{ka}{2}\right) = -\eta Ce^{-\eta a/2}$

$\frac{\cancel{B}k\sin(\,)}{\cancel{B}\cos(\,)} = \frac{\eta \cancel{Ce^{-\eta a/2}}}{\cancel{Ce^{-\eta a/2}}}$

$k\tan\left(\frac{ka}{2}\right) = \eta$

$\Rightarrow$ EVEN $k\tan(ka/2) = \eta$

ODD $-k\cot g(ka/2) = \eta$

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

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

$y = \frac{ka}{2}$ $R = \sqrt{\frac{2mV_0}{\hbar^2}\left(\frac{a}{2}\right)^2}$

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

$\frac{ka}{2} \to y$, $\frac{ka}{2} \to y$, $\frac{\eta a}{2} \to \eta$

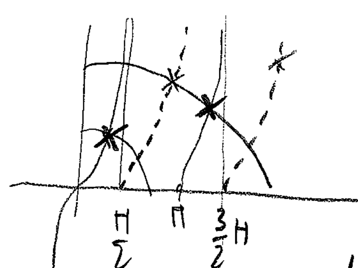
$\eta^2\left(\frac{a}{2}\right)^2 = \underbrace{\frac{2m}{\hbar^2}V_0\left(\frac{a}{2}\right)^2}_{R^2} - \underbrace{k^2\left(\frac{a}{2}\right)^2}_{y^2}$

$\Downarrow$

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

CYCLE radius R.

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

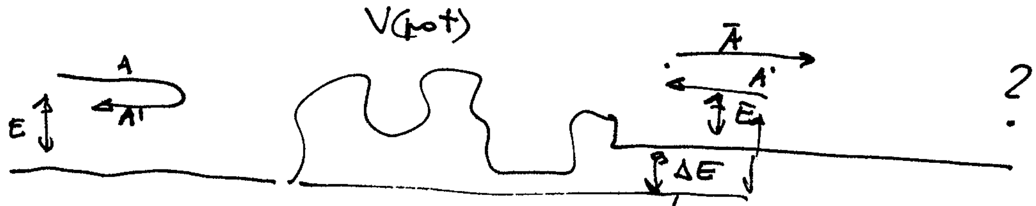


fix (V_0, a)
$\Rightarrow R$

get $y_n \Rightarrow \underline{k_n}$!!

φM4

TRANSMISSION MATRIT



$$\psi = A e^{ik_i x} + A' e^{-ik_i x} \qquad \psi = \bar{A} e^{i\bar{k}_T x} + \bar{A}' e^{-i\bar{k}_T x}$$

$$k_i = \sqrt{\frac{2mE}{\hbar^2}} \qquad \cancel{\text{if } \Delta E = 0 \Rightarrow k =} \qquad \bar{k}_T = \sqrt{\frac{2m(E-\Delta E)}{\hbar^2}}$$

$$\bar{A} = F(k_i)A + F'(k_i)A'$$
$$\bar{A}' = G(k_i)A + G'(k_i)A' \Rightarrow M(k) = \begin{pmatrix} F(k) & F'(k) \\ G(k) & G'(k) \end{pmatrix}$$

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

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

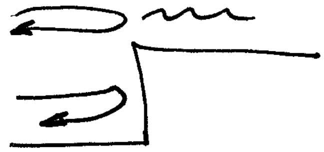
$$T \text{ transmission } (k) \equiv \left| \frac{\bar{A}(k)}{A(k)} \right|^2 = \frac{1}{|F(k)|^2} \qquad \text{if } \bar{A}' = 0$$

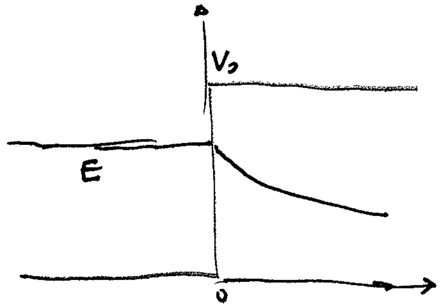
$$R + T = 1$$
conservation of probability

If $\Delta E = 0$, symmetrical or not
$\Rightarrow$ R, T from Right $\Longleftrightarrow$ TR from left

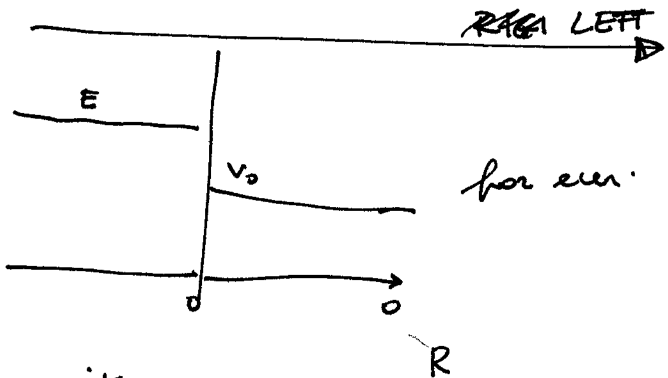
PMAS

POTENTIAL STEP





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



for ever.

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

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

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

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

$\psi_T = \bar{A} e^{ik_T x} + 0$ nothing at right

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

$\psi'(0) = ik_i A - ik_i A' = ik_T \bar{A}$

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

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

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

CLASSIC
$R = 0 \quad \xrightarrow{E \gg V_0}$
$T = 1$

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

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

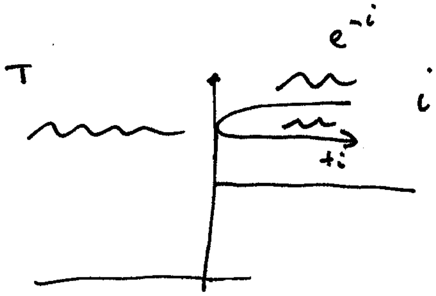
$\Rightarrow \quad \frac{A'}{A} = \frac{k_I - k_T}{k_I + k_T} \Rightarrow$

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

$\Rightarrow \quad \underline{\underline{T = 1 - R}}$

QM 6

RIGHT TO LEFT



$$\psi_i = A e^{-ik_i x} + A' e^{ik_i x}$$

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

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

$$T = 1 - R$$

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

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

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

$$\psi'(0) = -ik_i A + A' i k_i = -ik_T \underbrace{\bar{A}}_{A+A'}$$

$$\Downarrow$$

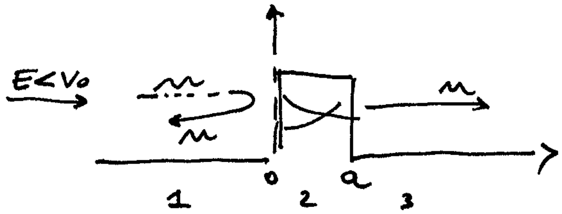
$$k_i (A' - A) = -k_T (A + A')$$

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

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

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

POTENTIAL WELL $V_0 \gtrless 0$ $E<V_0$ classic $\frac{R=1}{T=0}$



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

$$\eta_2 = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$$\psi_1 = Ae^{ikx} + A'e^{-ikx}$$
$$\psi_2 = Be^{\eta x} + B'e^{-\eta x}$$
$$\psi_3 = \bar{A}e^{ikx}$$

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

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

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

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

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

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

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

$$\underbrace{B'}_{=B^*} = \cancel{\ } \frac{-ik(A-A') + \eta(A+A')}{2\eta}$$

$$\cancel{\psi(a)} = \eta\left(\frac{Be^{\eta a} + B'e^{-\eta a}}{\cancel{e^{ika}}}\right) = \left(\frac{\eta(Be^{\eta a} - B'e^{-\eta a})}{ik\cancel{e^{ika}}}\right) \Big/ \eta$$

$\Rightarrow \cancel{B}$

QMA8

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

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

solve $\Rightarrow$

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

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

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

$$\frac{e^{x}+e^{-x}}{2} = \cosh x$$

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

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

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

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

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

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

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

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

QMA 9

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

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

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

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

$+$

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

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

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

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

if $\eta a >>> 1$ $\quad T \simeq 16\gamma(1-\gamma)e^{-2\eta a}$ $\quad E < V_0$

$\gamma = E/V_0 \longrightarrow$ Never 0!!

if $E > V_0$

$E > V_0$

$e^{\pm ikx}, e^{\pm i\varkappa x}, e^{ikx}$

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

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

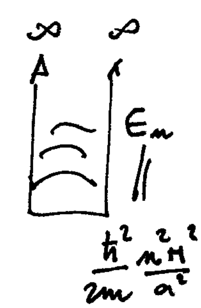
$\varkappa = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

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

$\sin^2(\varkappa a) = 0$ if $\varkappa a = n\pi$

$\varkappa^2 a^2 = n\pi$

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



QMA 6

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

$E = V_0 + n^2\frac{\pi^2\hbar^2}{2ma^2} = V_0 +$ Energy INFINITE WELL

THEORY OF MEASURE

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

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

what was the state of the system?

was a general state

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

measure E

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

eigen vector.

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

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

$$\Rightarrow E = \sum_{ij} a_i^* a_j^* E_j \underbrace{\int \psi_i \psi_j \, dx}_{1 = \delta_{ij}} =$$

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

a_n = scalar product of ψ_n and ψ

$\Rightarrow$ how much ψ_n is inside ψ

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

OR $(\psi_n)^* (\psi)$

$$\langle E_{\text{meas}} \rangle = \sum_n |a_n|^2 E_n$$

one of the outcomes

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

E_n as measure!