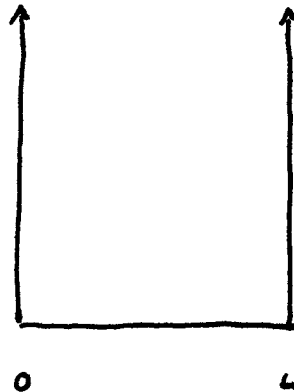


Lecture 9

INFINITE SQUARE WELL

"PARTICLE IN A BOX"



SOLVE TISE \Rightarrow STATIONARY STATES (TI)

\Downarrow
TIME-DEPENDENT STATES

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

$$\frac{d^2 \psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0$$

$$\frac{d^2 \psi}{dx^2} + K^2 \psi = 0$$

$$\Rightarrow A e^{iKx} + B e^{-iKx}$$

$$\sqrt{2mE/\hbar^2} = K$$

GENERAL SOLUTION

GENERAL SOLUTION

+

\Rightarrow SPECIFIC SOLN'S

BOUNDARY CONDITIONS

$$\psi(0) = 0 \Rightarrow A \sin(kx)$$

$$\psi(L) = 0 \Rightarrow A \sin\left(\frac{n\pi}{L}x\right)$$

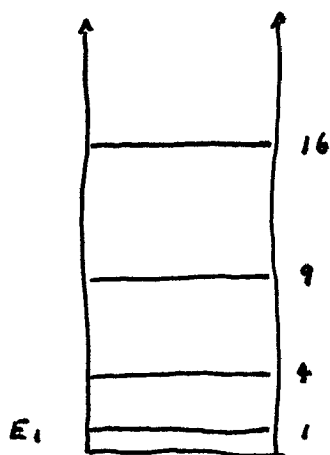
$$A \sin(k_n x)$$

$$k_n = \frac{n\pi}{L}$$

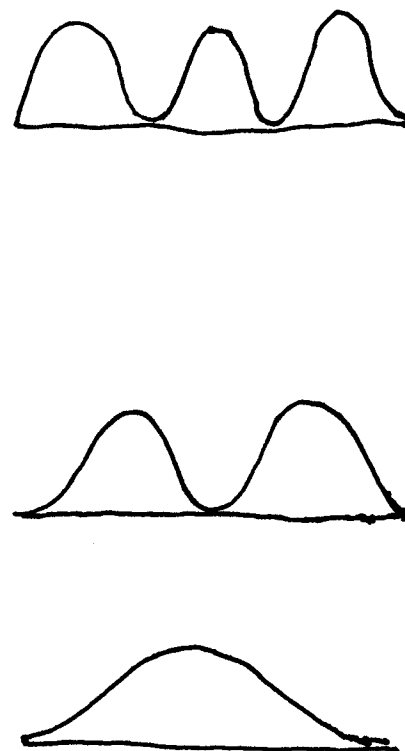
NORMALIZED STATIONARY STATES

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

$$k_n = \frac{n\pi}{L} \Rightarrow E_n = \frac{\hbar^2 k_n^2}{2m} = \left(\frac{\pi^2 \hbar^2}{2mL^2}\right) n^2 = E_1 n^2$$



PROB DIST



$$P_1(x) = \psi_1^*(x) \psi_1(x) = |\psi_1(x)|^2$$

$$E_n \sim n^2 / L^2$$

The larger the well, the lower the energy

The higher the quantum number n , the higher the energy

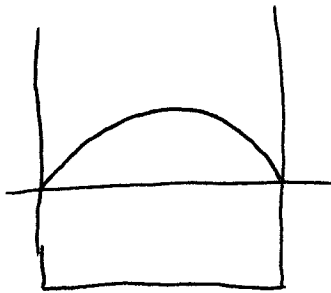
$$E = KE + PE$$

The potential energy for the square well is the same everywhere except at the boundaries where it is infinite. Consequently, the wavefunction must be zero at the boundaries.

The kinetic energy for the square well is proportional to the curvature of the wavefn.

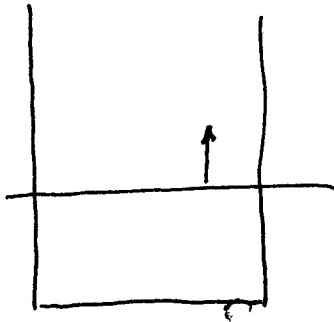
The ground state wavefunction has the minimum curvature---that is not zero everywhere and is zero at its ends.

IF YOU MEASURE POSITION



BEFORE

$\psi_1(x)$ eigenfunction of energy



AFTER

eigenfunction of position

NRQM: This is instantaneous

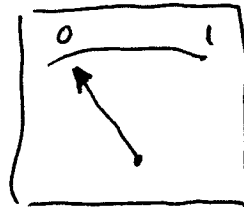
RQM: NOT INSTANTANEOUS



MICRO WORLD

REVERSIBLE

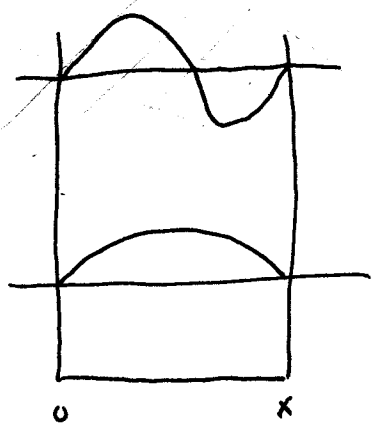
BOHR'S STRAIGHT LINE



MACRO WORLD

IRREVERSIBLE

MEASURE POSITION ?

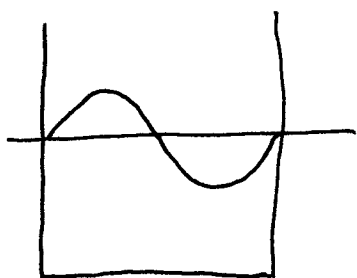


FIRST STATIONARY STATE $\psi_1(x)$

$$PROB(x) dx = P(x) dx = |\psi_1(x)|^2 dx$$



$P(x)$ is stationary

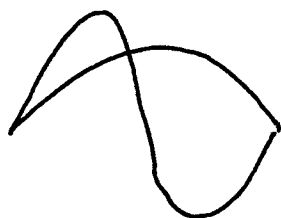


SECOND STATIONARY STATE $\psi_2(x)$

$$P(x) dx = |\psi_2(x)|^2 dx$$



$P(x)$ is stationary



SUPERPOSITION STATE

$$\psi(x,0) = (\psi_1(x) + \psi_2(x)) \frac{1}{\sqrt{2}}$$



$\psi(x,0)$



NOW $P(x)$ is not stationary!

$$P(x,0) = |\psi(x,0)|^2$$

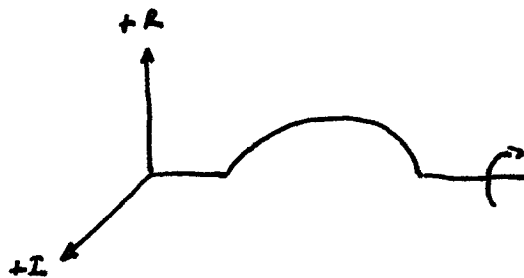
TIME-DEPENDENCE OF THE ENERGY EIGENKETS

$$|E_m(t)\rangle = e^{-iE_m t/\hbar} |E_m(0)\rangle$$

TIME-DEPENDENCE OF THE STATIONARY STATES

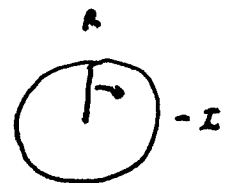
$$\psi_m(x,t) = e^{-iE_m t/\hbar} \psi_m(x)$$

IN POSITION SPACE



$$\omega_1 = E_1/\hbar$$

CLOCK HAND



$$\omega_2 = E_2/\hbar = 4E_1/\hbar$$

$$\omega_2 = 4\omega_1$$



$$\omega_3 = E_3/\hbar = 9\omega_1$$

THE QUANTUM BABY RATTLE

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} |E_1\rangle + \frac{1}{\sqrt{2}} |E_2\rangle$$

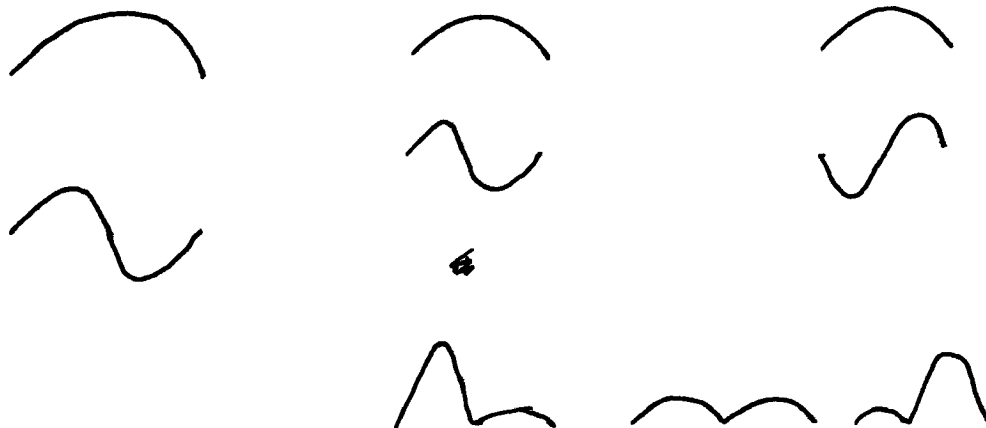
$$\psi(x,0) = \frac{1}{\sqrt{2}} \psi_1(x) + \frac{1}{\sqrt{2}} \psi_2(x)$$

TD

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} |E_1\rangle e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{2}} |E_2\rangle e^{-iE_2 t/\hbar}$$

$$\psi(x,t) = \frac{1}{\sqrt{2}} \psi_1(x) e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{2}} \psi_2(x) e^{-iE_2 t/\hbar}$$

CYCLIC BEHAVIOR: in phase, perp, 180° out, perp



50:50 SUPERPOSITION STATE

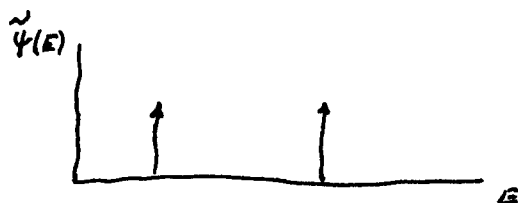
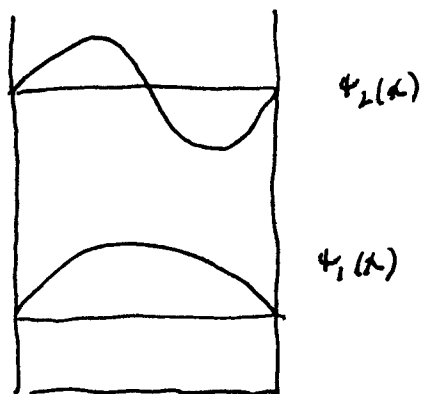
$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} |E_1\rangle + \frac{1}{\sqrt{2}} |E_2\rangle$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} |E_1\rangle e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{2}} |E_2\rangle e^{-iE_2 t/\hbar}$$

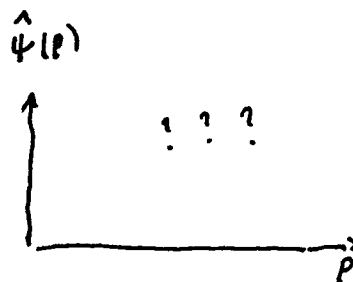
$$\langle x | \psi(x, t) = \frac{1}{\sqrt{2}} \psi_1(x) e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{2}} \psi_2(x) e^{-iE_2 t/\hbar}$$

$$\langle p | \hat{\psi}(p, t) = \frac{1}{\sqrt{2}} \hat{\psi}_1(p) e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{2}} \hat{\psi}_2(p) e^{-iE_2 t/\hbar}$$

$$\langle E | \tilde{\psi}(E, t) = \frac{1}{\sqrt{2}} \delta(E - E_1) e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{2}} \delta(E - E_2) e^{-iE_2 t/\hbar}$$



TWO QUESTIONS:



$\langle x(t) \rangle$

IF YOU MEASURE

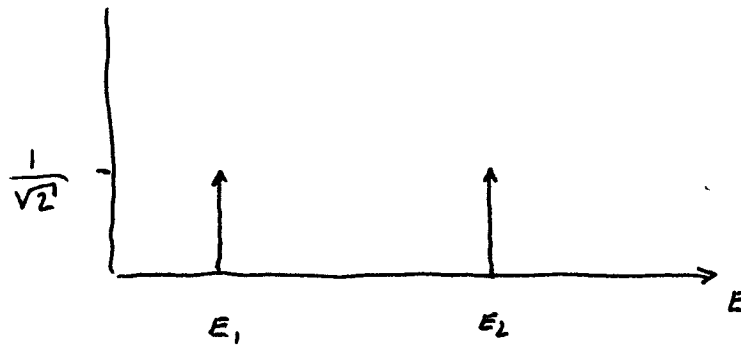
ENERGY

POSSIBLE

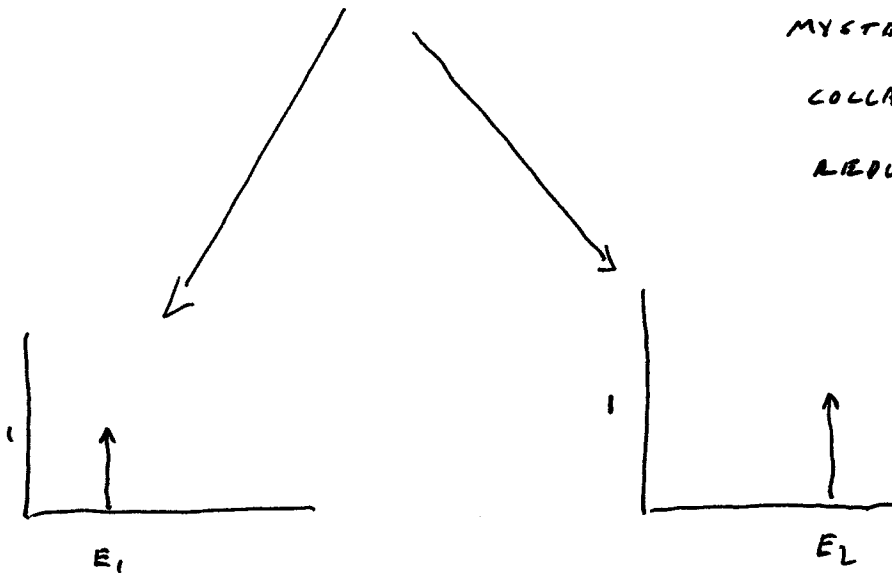
RESULTS : EIGENVALUES OF THE HAMILTONIAN

EIGEN ENERGIES

PROBABILITIES : HOW MUCH OF THAT EIGENSTATE IS IN $|\psi\rangle$



MYSTERIOUS QUANTUM JUMP
COLLAPSE OF THE WAVEFN
REDUCTION OF THE STATE
VECTOR



MYSTERIOUS BECAUSE :

MEASURE ENERGY \Rightarrow WHAT ARE POSSIBLE RESULTS?

WHAT ARE THE ASSOCIATED PROBS?

COMMON SENSE

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} |E_1\rangle + \frac{1}{\sqrt{2}} |E_2\rangle$$

EQUAL MIXTURE OF E_1 AND E_2

EQUAL PROB OF E_1 AND E_2

TOTAL PROB = 1

$$\text{PROB}(E_1) = \frac{1}{2}$$

$$\text{PROB}(E_2) = \frac{1}{2}$$

$$\left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$$

$$\text{PROB} = |a_j|^2$$

$$\text{if } \sum_j |a_j|^2 = 1$$

FORMAL METHOD

MEASURE ENERGY

POSSIBILITIES : EIG'S OF H

$$E_1, E_2, E_3, \dots$$

PROB OF EACH ONE: 50% E_1 50% E_2

$$\begin{aligned} \text{PROB}(E_1) &= \left| \langle E_1 | \psi(t) \rangle \right|^2 \\ &= \left| \left\langle E_1 \left| \left(\frac{1}{\sqrt{2}} |E_1\rangle e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{2}} |E_2\rangle e^{-iE_2 t/\hbar} \right) \right\rangle \right|^2 \\ &= \left| \frac{1}{\sqrt{2}} e^{-iE_1 t/\hbar} \right|^2 = \frac{1}{2} \end{aligned}$$

$$\text{PROB}(E_1) = \left| \int_0^a \psi_1^*(x) \left(\frac{1}{\sqrt{2}} \psi_1(x) e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{2}} \psi_2(x) e^{-iE_2 t/\hbar} \right) dx \right|^2$$

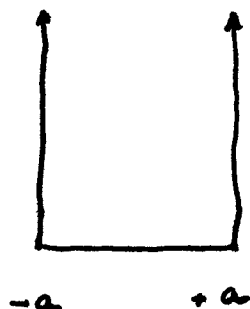
$$\begin{aligned} &= \left| \frac{1}{\sqrt{2}} \frac{2}{a} \int_0^a \sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{\pi}{a} x\right) e^{-iE_1 t/\hbar} dx \right. \\ &\quad \left. + \frac{1}{\sqrt{2}} \frac{2}{a} \int_0^a \sin\left(\frac{2\pi}{a} x\right) \sin\left(\frac{2\pi}{a} x\right) e^{-iE_2 t/\hbar} dx \right|^2 \end{aligned}$$

$$= \left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2} \Rightarrow 50\%$$

WORKS FOR ANY

$$f(x) = \psi(x, 0)$$

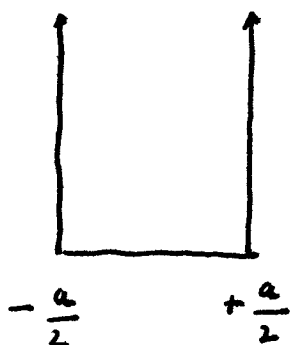
THREE CONVENTIONS FOR THE SQUARE WELL



$$\psi_n(x) = \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi}{2a} x\right) \quad n \text{ odd}$$

$$= \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi}{2a} x\right) \quad n \text{ even}$$

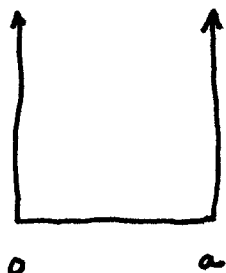
$$E_n = \left(\frac{\hbar^2 \pi^2}{8ma^2}\right) n^2 \quad L = 2a$$



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

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

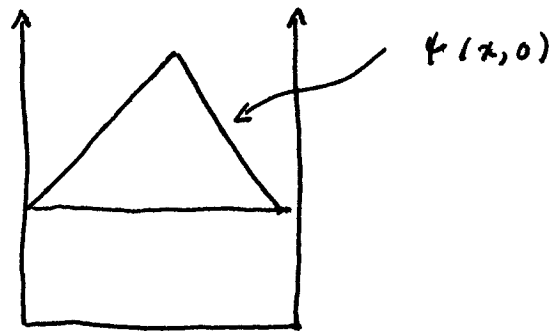
$$E_n = \left(\frac{\hbar^2 \pi^2}{2ma^2}\right) n^2$$



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

$$E_n = \left(\frac{\hbar^2 \pi^2}{2ma^2}\right) n^2$$

TIME - DEPENDENCE OF AN ARBITRARY STATE



FOUR-STEP PLAN

(1) DIAGONALIZE H

(2) EXPAND $|\psi(0)\rangle$

(3) WRITE DOWN $|\psi(t)\rangle$

(4) CALCULATE EVERYTHING $\langle x \rangle \quad \Delta x$

$\langle p \rangle \quad \Delta p$

$\langle E \rangle \quad \Delta E$

\vdots

$$|\psi(0)\rangle = \sum_m |E_m\rangle \langle E_m | \psi(0) \rangle$$

$$|\psi(t)\rangle = \sum_m e^{-iE_m t/\hbar} |E_m\rangle \underbrace{\langle E_m | \psi(0) \rangle}_{a_m}$$

$$|\psi(t)\rangle = \sum_m a_m |E_m\rangle e^{-iE_m t/\hbar}$$

in x basis

$$\psi(x, t) = \sum_m a_m \psi_m(x) e^{-iE_m t/\hbar}$$

EXPANSION COEFFICIENTS

$$a_m = \langle E_m | \psi(0) \rangle = \langle E_m | I | \psi(0) \rangle$$

$$= \int \underbrace{\langle E_m | x \rangle}_{\psi_m^*(x)} \underbrace{\langle x | \psi(0) \rangle}_{\psi(x,0)} dx$$

$$a_m = \int \psi_m^*(x) \psi(x,0) dx$$

CARTOON VERSION



||

SYMMETRY \Rightarrow ONLY ODD TERMS

a_1



+

a_2



+

a_3



+

a_4



+

a_5



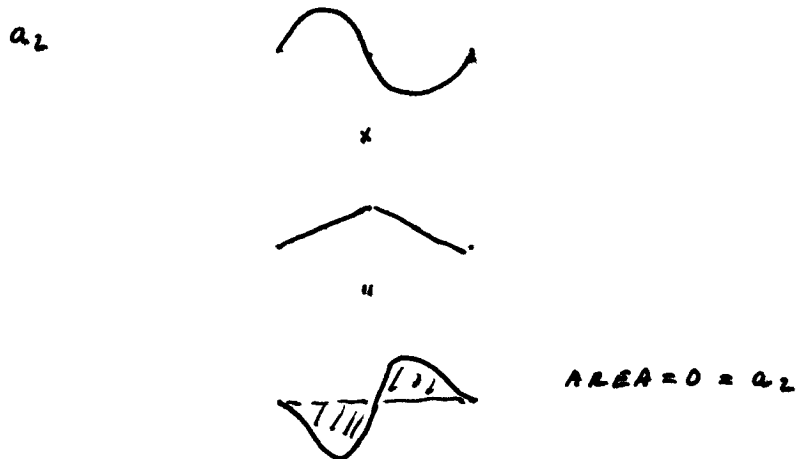
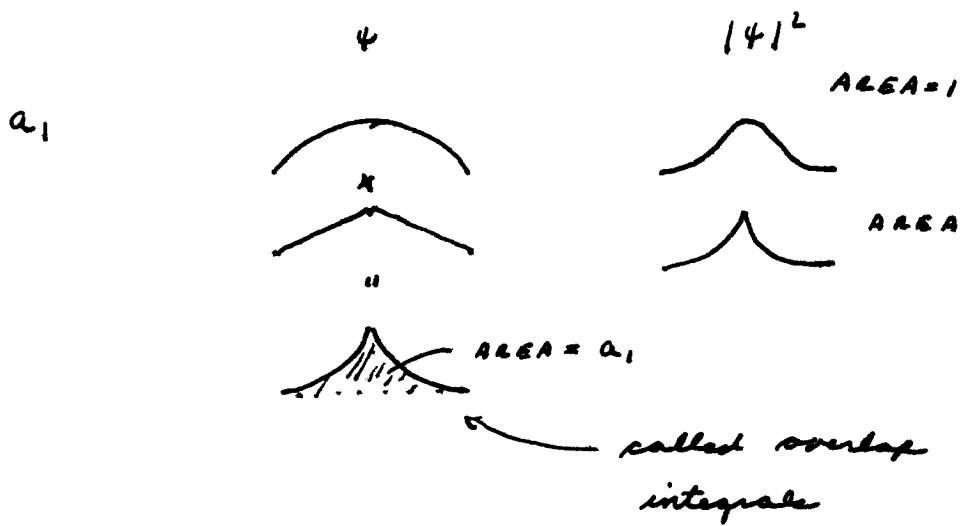
+

\vdots

TO CALCULATE THE EXPANSION COEFFS

$$a_m = \int_0^L \psi_m^*(x) \psi(x,0) dx$$

$$= \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \psi(x,0) dx$$



12-760	200 SHELLEY DRIVE	5 SUITES
42-435	200 SHELLEY DRIVE	5 SUITES
42-482	200 SHELLEY DRIVE	5 SUITES
42-489	200 SHELLEY DRIVE	5 SUITES

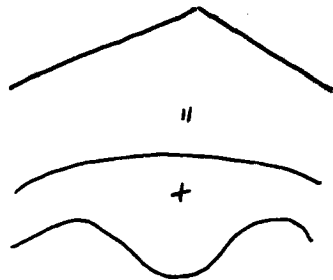
τ_1

$$T_3 = \frac{T_1}{9}$$

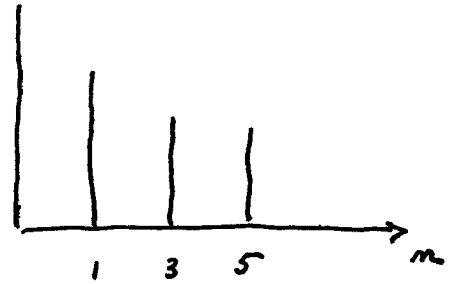
$$T_5 = \frac{T_1}{25}$$

\Rightarrow RECURRENCE TIME = T_1 !

FOR THE SQUARE WELL



FOURIER
SERIES

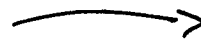


a_m 's are the FOURIER SERIES EXPANSION
COEFFS! DISCRETE

FOR THE FREE PARTICLE



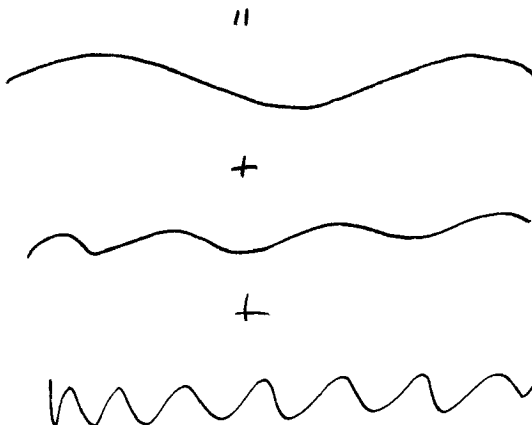
Gaussian



FOURIER
TRANSFORM



Gaussian



a_m 's are given
by the Fourier
transform coeffs

CONTINUOUS

SHOW MOVIES HERE! ?

EXPECTATION VALUES

IF $[H, Q] = 0$ THEN $\langle Q \rangle$ and $\langle Q^2 \rangle$ are constant

SINCE $[H, H] = 0$ $\langle H \rangle = \langle E \rangle$ constant

$\langle H^2 \rangle = \langle E^2 \rangle$ constant

FOR THE QUANTUM RATTLE

$$\langle E(0) \rangle = \langle \psi(0) | H | \psi(0) \rangle$$

$$= \frac{1}{\sqrt{2}} \left(\langle E_2 | + \langle E_1 | \right) H \frac{1}{\sqrt{2}} \left(| E_1 \rangle + | E_2 \rangle \right)$$

$$= \frac{1}{2} (E_1 + E_2)$$

$$= \frac{5}{2} E_1 \quad E_2 = 4 E_1$$

$$\langle E(t) \rangle = \langle \psi(t) | H | \psi(t) \rangle$$

$$= \frac{1}{\sqrt{2}} \left(\langle E_2 | e^{+i E_2 t / \hbar} + \langle E_1 | e^{+i E_1 t / \hbar} \right) H$$

$$\frac{1}{\sqrt{2}} \left(| E_1 \rangle e^{-i E_1 t / \hbar} + | E_2 \rangle e^{-i E_2 t / \hbar} \right)$$

$$= \frac{5}{2} E_1$$

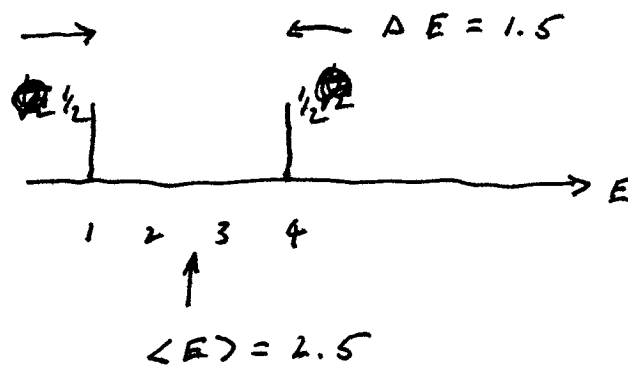
$$\begin{aligned}
 \langle \psi | H^2 | \psi \rangle &= (\langle E_L | + \langle E_1 |) \frac{1}{\sqrt{2}} H^2 \frac{1}{\sqrt{2}} (|E_1\rangle + |E_L\rangle) \\
 &= \frac{1}{2} (\langle E_L + \langle E_1 |) (E_1^2 |E_1\rangle + E_L^2 |E_L\rangle) \\
 &= \frac{1}{2} E_1^2 + \frac{1}{2} E_L^2
 \end{aligned}$$

since $E_L = 4E_1$

$$\begin{aligned}
 &= \left(\frac{1}{2} + \frac{16}{2} \right) E_1^2 \\
 &= \frac{17}{2} E_1^2 \quad \text{TI}
 \end{aligned}$$

$$\begin{aligned}
 \Delta H &= \sqrt{(\langle H^2 \rangle - \langle H \rangle^2)} \\
 &= \sqrt{\frac{17}{2} E_1^2 - \left(\frac{5}{2} E_1 \right)^2} \\
 &= \sqrt{\frac{34 - 25}{4} E_1^2} \quad \text{TI}
 \end{aligned}$$

$$= \frac{3}{2} E_1$$



POSITION: $\langle x \rangle$ $\langle x^2 \rangle$ Δx

$$[x, H] = x \left(\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) - \left(\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) x$$

IN GENERAL

$$[x, H] \neq 0$$

$$[x^2, H] \neq 0$$

BUT FOR THE STATIONARY STATES

$$\begin{aligned} \langle E_m | (xH - Hx) | E_m \rangle &= \langle E_m | (-Hx + xH) | E_m \rangle \\ &= \langle E_m | (-E_m x + x E_m) | E_m \rangle \\ &= 0 \end{aligned}$$

$$\langle x(t) \rangle = \langle \psi(t) | x | \psi(t) \rangle$$

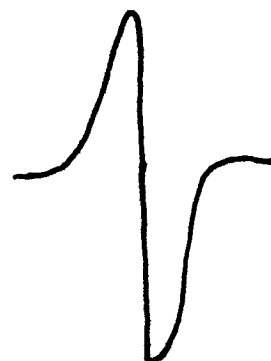
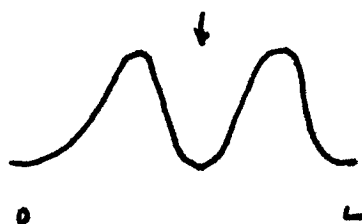
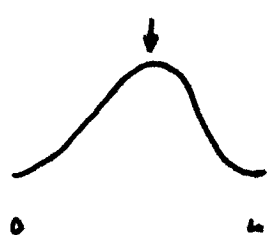
$$= \frac{1}{\sqrt{2}} \left(\langle E_1 | e^{+iE_1 t/\hbar} + \langle E_2 | e^{+iE_2 t/\hbar} \right) x$$

$$\frac{1}{\sqrt{2}} \left(|E_1\rangle e^{-iE_1 t/\hbar} + |E_2\rangle e^{-iE_2 t/\hbar} \right)$$

$$\begin{aligned} &= \frac{1}{2} \int x dx \left(\psi_1^*(x) e^{i\omega_1 t} + \psi_2^*(x) e^{i\omega_2 t} \right) \\ &\quad \left(\psi_1(x) e^{-i\omega_1 t} + \psi_2(x) e^{-i\omega_2 t} \right) \end{aligned}$$

$$\begin{aligned}
 \langle x(t) \rangle = \int_0^L x \, dx \left[\frac{1}{2} |\psi_1(x)|^2 + \frac{1}{2} |\psi_2(x)|^2 \right. \\
 \left. + \psi_1(x) \psi_2(x) \cos(\Omega t) \right]
 \end{aligned}$$

$$\Omega = \omega_2 - \omega_1 = (E_2 - E_1)/\hbar = 3E_1/\hbar = 3\omega_1$$



OSCILLATING

DOING THE INTEGRALS



x



||

?



x



||

?



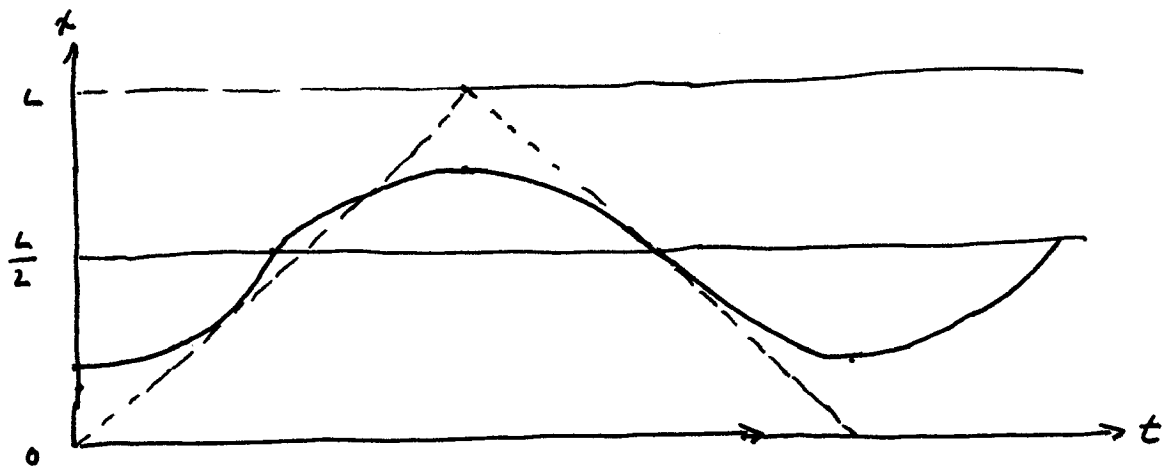
x



||

?

$$\langle \psi(t) | x | \psi(t) \rangle = \langle x(t) \rangle = \frac{L}{2} - \frac{16L}{9\pi^2} \cos(\Omega t)$$



quantum particle feels the walls
sooner than the classical point
particle

$$\frac{2}{L} \int_0^L \sin\left(\frac{\pi}{L} x\right) x \sin\left(\frac{2\pi}{L} x\right) dx = -\frac{16L}{9\pi^2}$$

EXPECTATION VALUES IN MOMENTUM SPACE

in general $[p, H] \neq 0$

for stationary states $[p, H] = 0$

$$\langle E_n | p H - H p | E_n \rangle$$

$$\langle E_n | -H p + p H | E_n \rangle$$

$$\langle E_n | -E_n p + p E_n | E_n \rangle$$

0

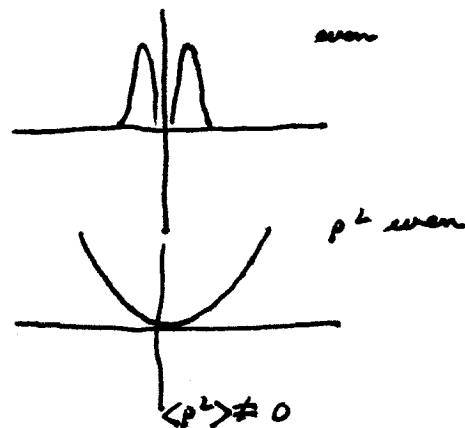
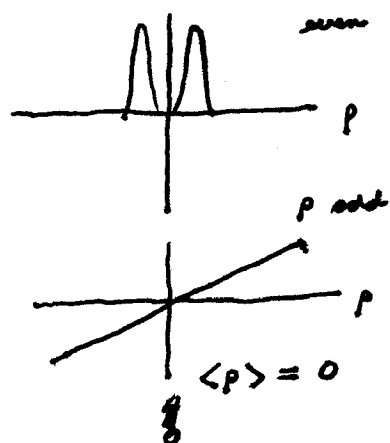
FOR THE ENERGY EIGENSTATES

$$\langle p \rangle = 0$$

$$\langle p^2 \rangle = \left(\frac{\hbar^2 \pi^2}{a^2} \right) n^2$$

$$\Delta p = \left(\frac{\hbar \pi}{a} \right) n$$

FROM COMPUTER SIMULATION



QM BABY RATTLE

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|E_1\rangle + |E_2\rangle)$$

$$\langle p(0) \rangle = \langle \psi(0) | p | \psi(0) \rangle$$

$$= \frac{1}{\sqrt{2}} (\langle E_1 | + \langle E_2 |) p \frac{1}{\sqrt{2}} (|E_1\rangle + |E_2\rangle)$$

in x -space

$$= \frac{1}{2} \int [\psi_1^*(x) + \psi_2^*(x)] -i\hbar \frac{d}{dx} [\psi_1(x) + \psi_2(x)] dx$$

in p -space

$$= \frac{1}{2} \int [\hat{\psi}_1^*(p) + \hat{\psi}_2^*(p)] p [\hat{\psi}_1(p) + \hat{\psi}_2(p)] dp$$

$$\langle p(t) \rangle = \langle \psi(t) | p | \psi(t) \rangle$$

similar to $\langle x(t) \rangle$

$$\int p dp \frac{1}{2} (|\hat{\psi}_1(p)|^2 + |\hat{\psi}_2(p)|^2) + [\hat{\psi}_1^*(p) \hat{\psi}_2(p) + \hat{\psi}_1(p) \hat{\psi}_2^*(p)] \sin(At)$$

WAVEFUNCTIONS IN MOMENTUM SPACE

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

$$\hat{\psi}_m(p) = FT(\psi_m(x))$$

$$= \sqrt{\frac{1}{2\pi\hbar}} \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-ipx/\hbar} dx$$

$$\frac{1}{2i} \left[e^{i(\dots)} - e^{-i(\dots)} \right]$$

$$= \frac{1}{2i} \sqrt{\frac{1}{2\pi\hbar}} \sqrt{\frac{2}{a}} \int_0^a \left[e^{i\left(\frac{n\pi}{a} - \frac{p}{\hbar}\right)x} - e^{-i\left(\frac{n\pi}{a} + \frac{p}{\hbar}\right)x} \right] dx$$

$$\frac{\exp\left(\frac{n\pi}{a} - \frac{p}{\hbar}\right)x - 1}{i\left(\frac{n\pi}{a} - \frac{p}{\hbar}\right)} - \frac{\exp\left(\frac{n\pi}{a} + \frac{p}{\hbar}\right)x - 1}{-i\left(\frac{n\pi}{a} + \frac{p}{\hbar}\right)}$$

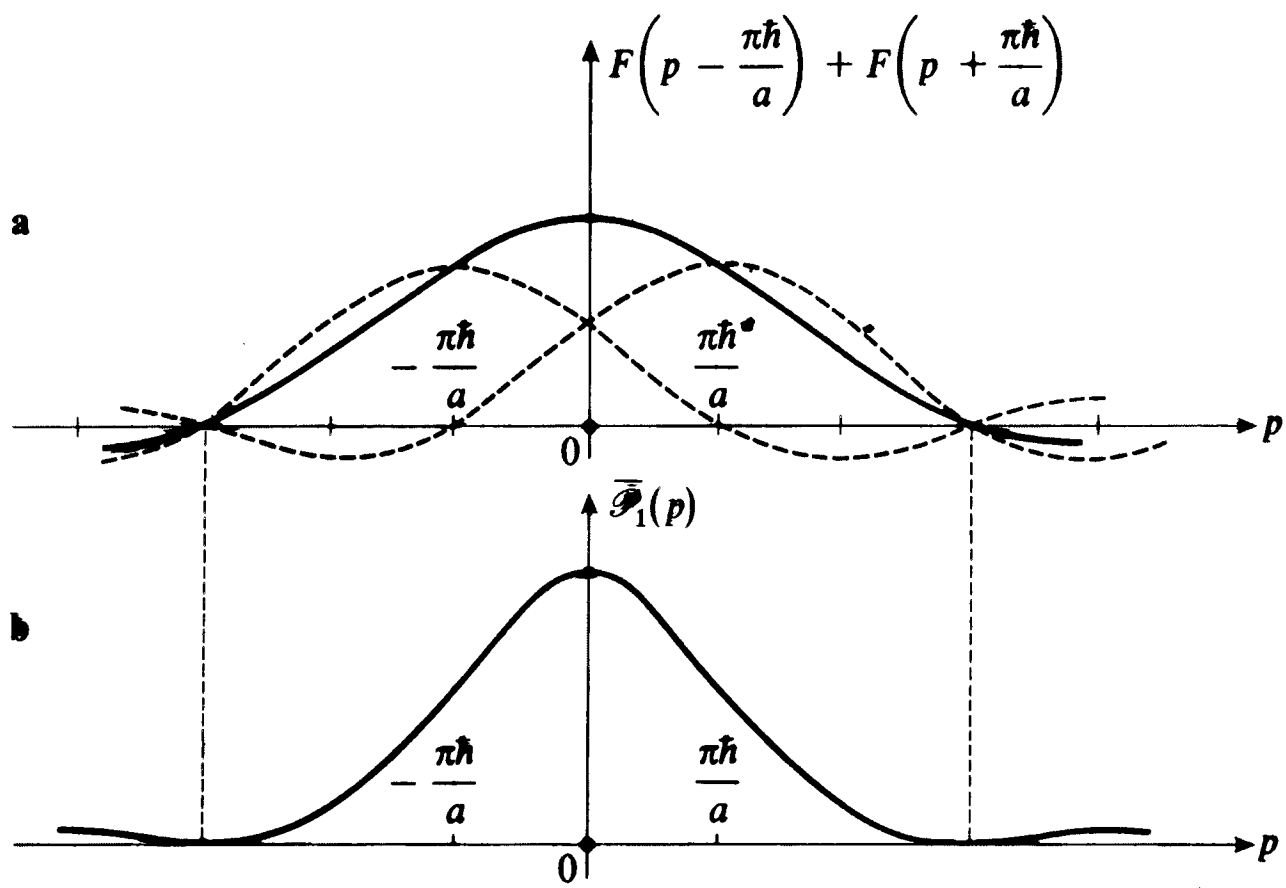
$$\hat{\psi}_m(p) = \frac{1}{2i} \sqrt{\frac{a}{\pi \hbar}} e^{i \left(\frac{n\pi}{2} - \frac{pa}{2\hbar} \right)}$$

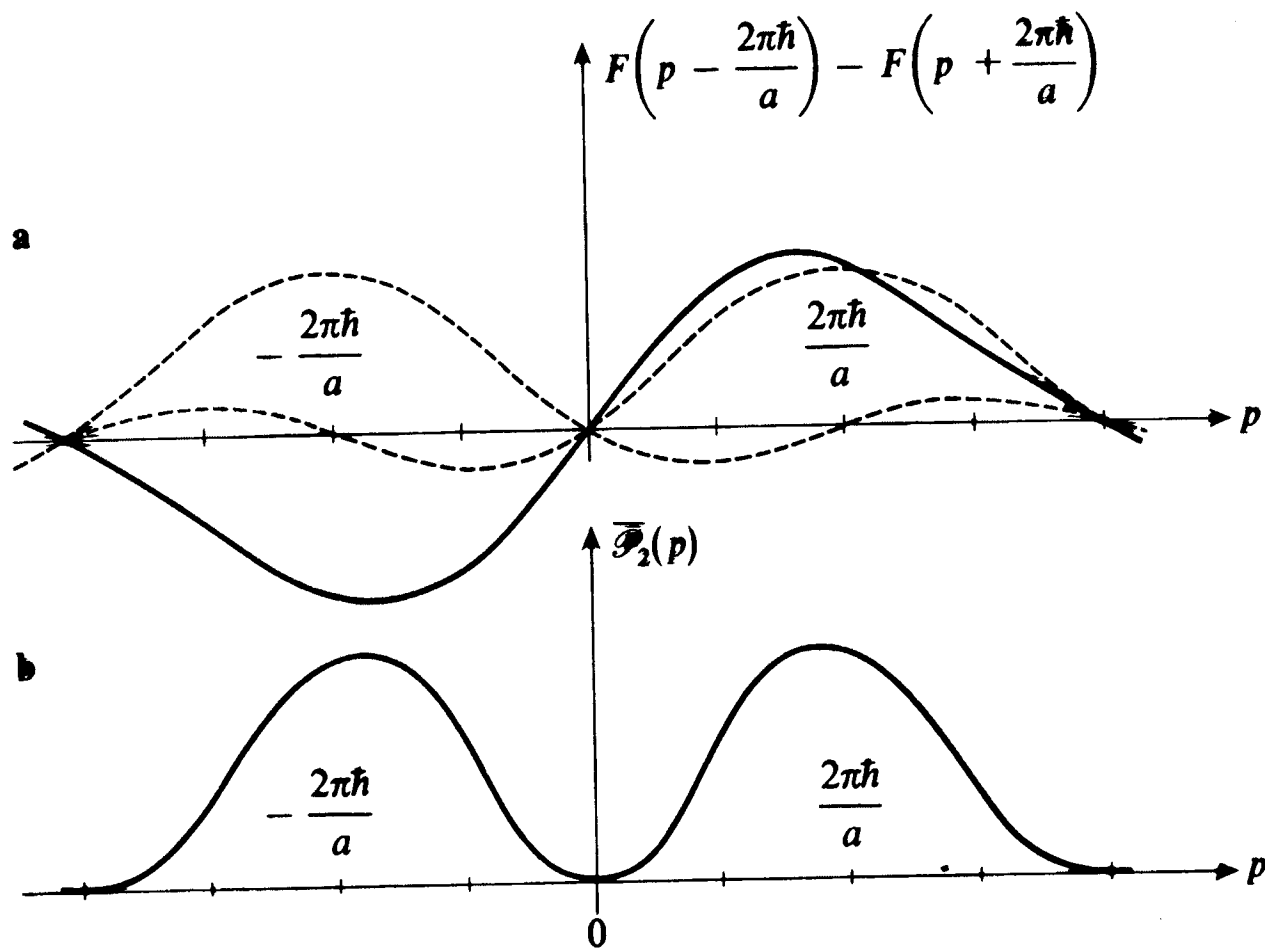
$$\times \left[F\left(p - \frac{n\pi \hbar}{a}\right) + (-1)^{n+1} F\left(p + \frac{n\pi \hbar}{a}\right) \right]$$

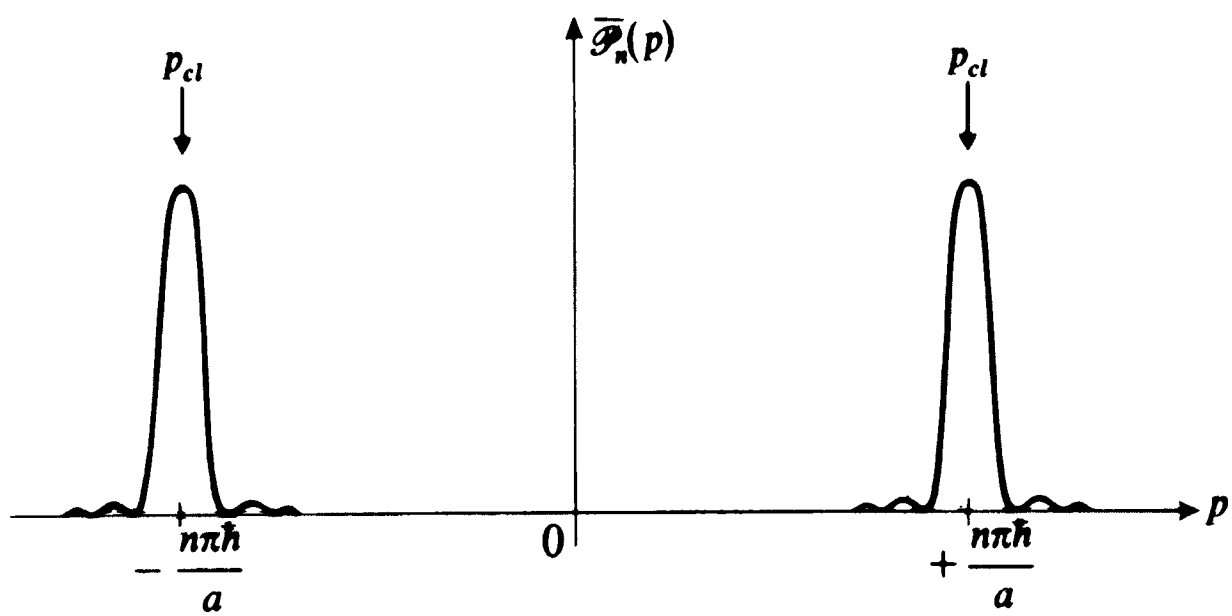
$$F(p) = \frac{\sin(pa/2\hbar)}{(pa/2\hbar)}$$

$$= \frac{\sin x}{x}$$

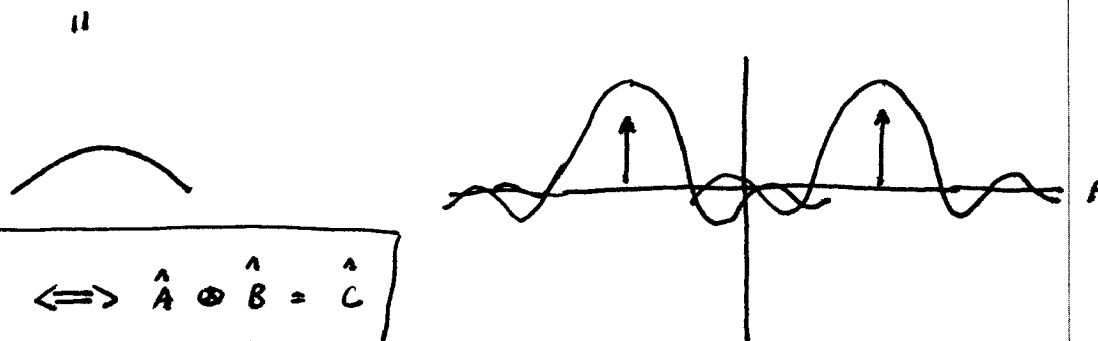
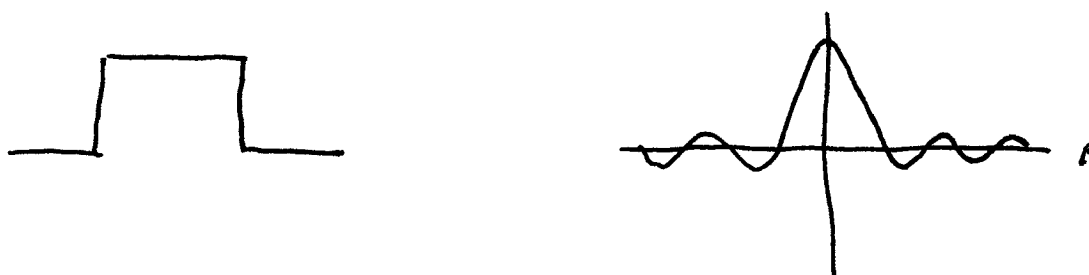
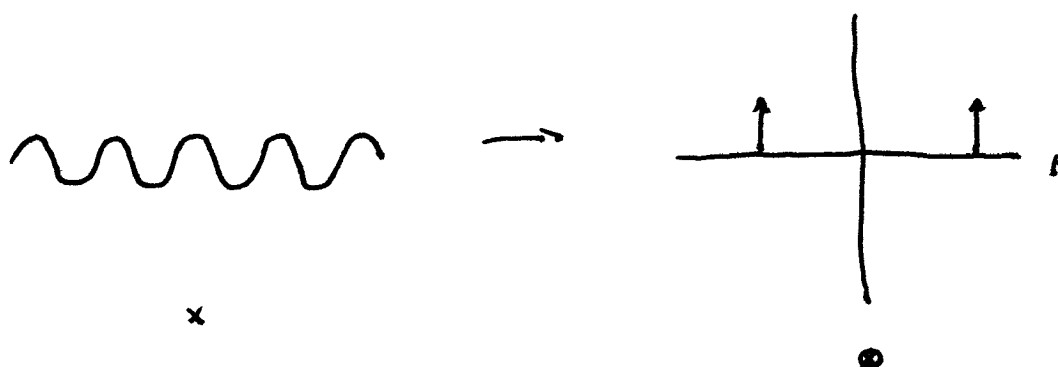
$$= \text{sinc}(x)$$







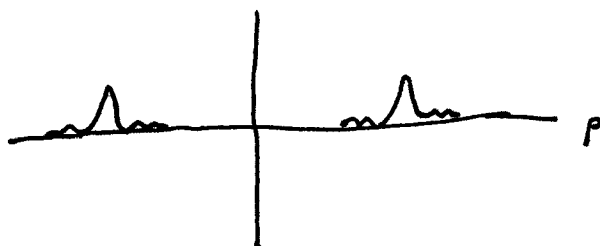
CARTOON VERSION



$$A \cdot B = C \iff \hat{A} \oplus \hat{B} = \hat{C}$$

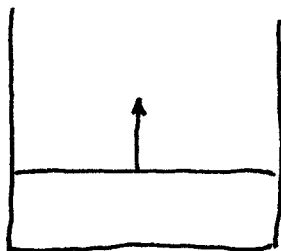
CONVOLUTION THEOREM

as $n \uparrow$, more and more like a ^{simple} standing wave



MEASURE x


FIND IN CENTER OF WELL



BY SYMMETRY \Rightarrow ONLY ODD n

 yes

 yes

 no

$$P(E_n) = \frac{2}{a} \quad n \text{ odd}$$

$$= 0 \quad n \text{ even}$$

$\Rightarrow \infty$ ENERGY

FINITE \times RESOLUTION

