Square Well Redux

Summarize

Three Conventions

Arbitrary State

Toy Model

- quantum baby rattle
- two energy eigenstates

Expectation Values

- energy
- position

Momentum Space

- wavefunctions
- probability distributions
- expectation values

GENERAL SOLUTION
+
BOUNDARY CONDITIONS $\Rightarrow$ SPECIFIC SOLN'S

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

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

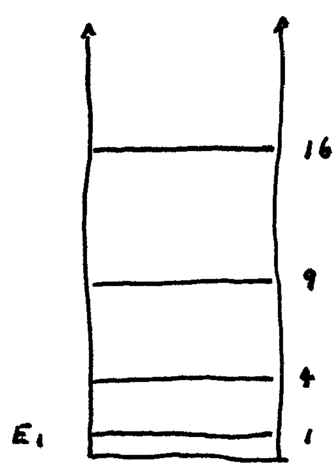
$$A \sin(k_n x)$$

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

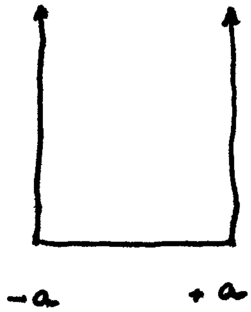
NORMALIZED STATIONARY STATES

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

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



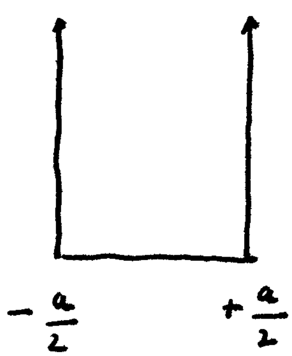
THREE CONVENTIONS FOR THE SQUARE WELL



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

$$= \sqrt{\frac{1}{a}}\,\sin\left(\frac{n\pi}{2a}x\right) \qquad n \text{ EVEN}$$

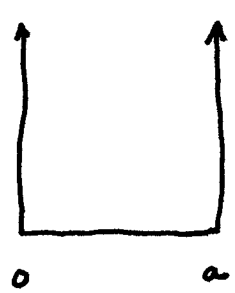
$$E_n = \left(\frac{\hbar^2\pi^2}{8ma^2}\right)n^2 \qquad L = 2a$$



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

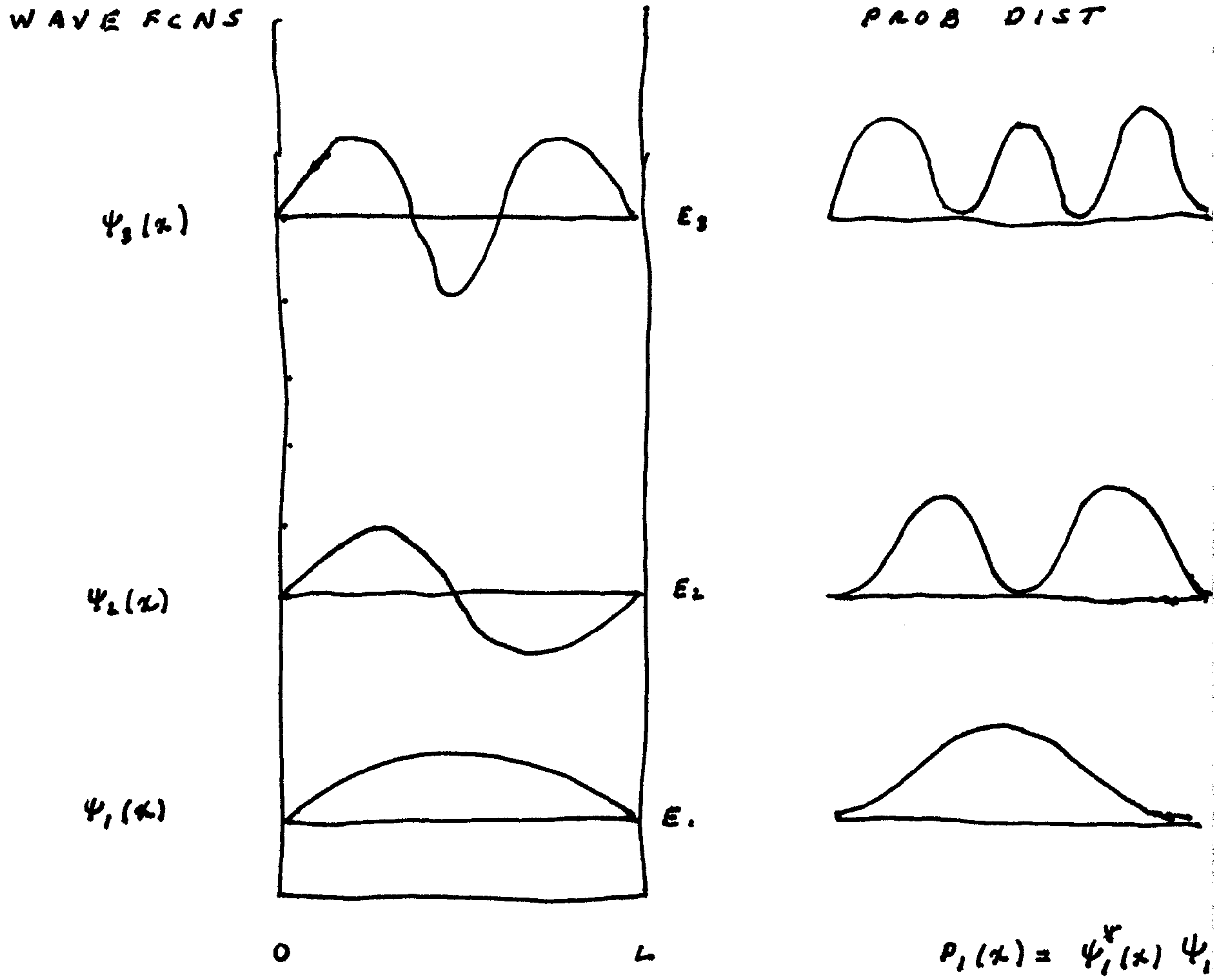
$$= \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi}{a}x\right) \qquad n \text{ even}$$

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



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

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



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

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

The larger the well, the lower the energy

The higher the quantum number n, the higher the energy

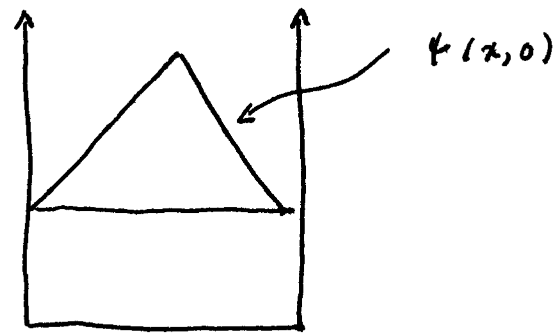
E = KE + PE

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 wavefcn.

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

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 $\quad \langle x \rangle \quad \Delta x$

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

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

$\vdots$

$$|\psi(0)\rangle = \sum_n |E_n\rangle \langle E_n | \psi(0)\rangle$$

$$|\psi(t)\rangle = \sum_n e^{-iE_n t/\hbar} |E_n\rangle \underbrace{\langle E_n | \psi(0)\rangle}_{a_n}$$

$$|\psi(t)\rangle = \sum_n a_n |E_n\rangle e^{-iE_n t/\hbar}$$

in x basis

$$\psi(x,t) = \sum_n a_n \psi_n(x) e^{-iE_n t/\hbar}$$

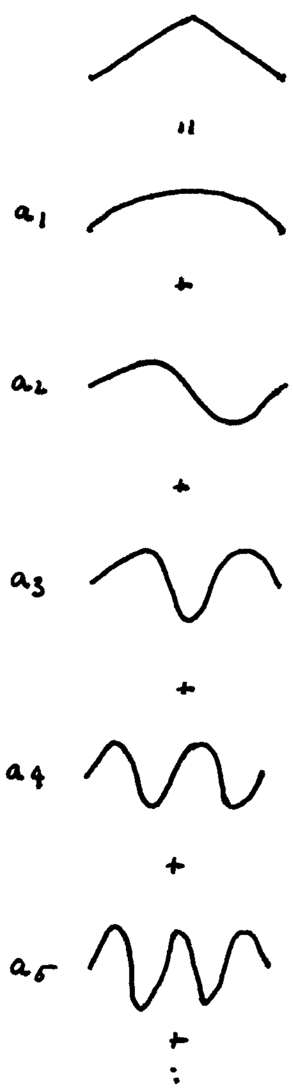
EXPANSION COEFFICIENTS

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

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

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

CARTOON VERSION



SYMMETRY => ONLY ODD TERMS

TO CALCULATE THE EXPANSION COEFFS

$$a_n = \int_0^L \psi_n^*(x)\ \psi(x,0)\ dx$$

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

ψ $\qquad\qquad$ $|\psi|^2$

AREA = 1

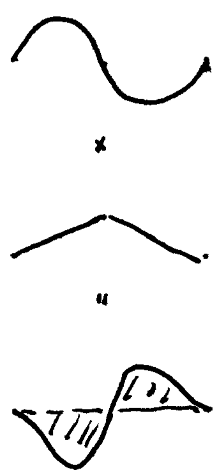
a_1

AREA

AREA = a_1

called overlap integrals

a_2

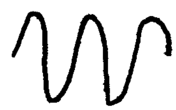


AREA = 0 = a_2

TIME - DEPENDENCE

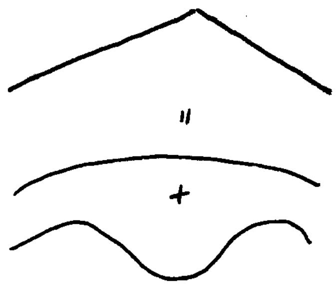
$\psi(x,t) = a_1 e^{-i\omega_1 t}$  T_1

$+ a_3 e^{-i\omega_3 t}$  $T_3 = \frac{T_1}{9}$

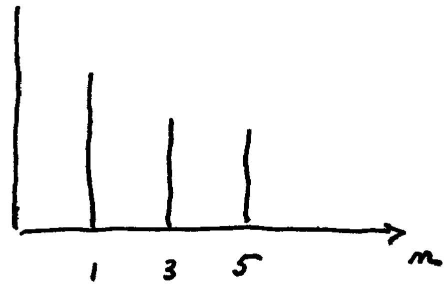
$+ a_5 e^{-i\omega_5 t}$  $T_5 = \frac{T_1}{25}$

$\Rightarrow$ RECURRENCE TIME $= T_1$!

FOR THE SQUARE WELL



FOURIER SERIES



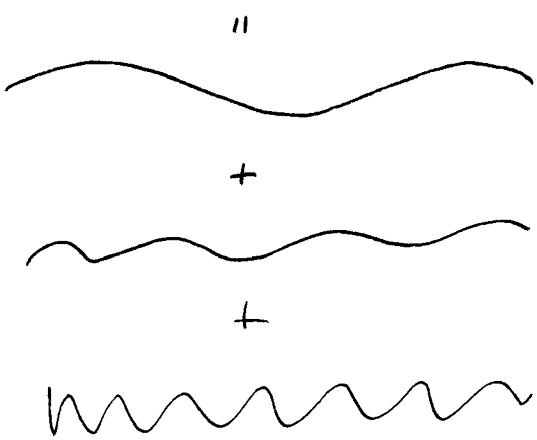
a_n's are the FOURIER SERIES EXPANSION COEFFS! DISCRETE

FOR THE FREE PARTICLE

Gaussian

FOURIER TRANSFORM

Gaussian

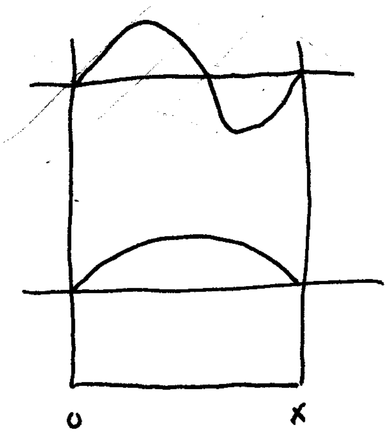


a_n's are given by the Fourier transform coeffs

CONTINUOUS

SHOW MOVIES HERE!?

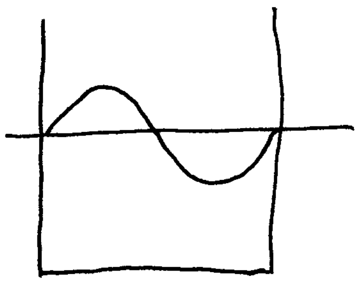
MEASURE POSITION ?



FIRST STATIONARY STATE $\psi_1(x)$

$$\text{PROB}(x)\,dx = P(x)\,dx = |\psi_1(x)|^2\,dx$$

$P(x)$ is stationary



SECOND STATIONARY STATE $\psi_2(x)$

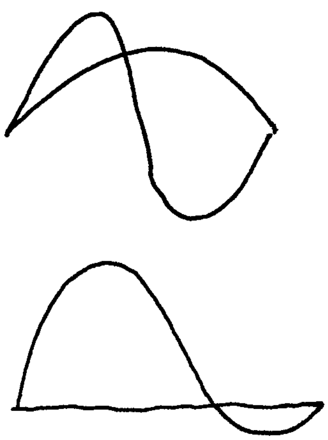
$$P(x)\,dx = |\psi_2(x)|^2\,dx$$

$P(x)$ is stationary

SUPERPOSITION STATE

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

NOW $P(x)$ is not stationary !



$\psi(x,0)$

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

TIME-DEPENDENCE OF THE ENERGY EIGENKETS

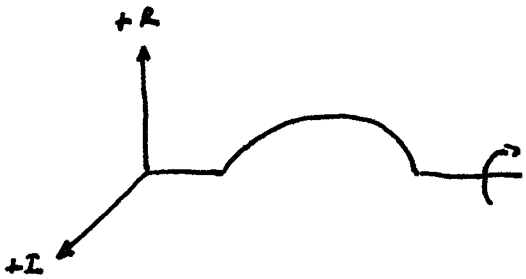
$$| E_m(t) \rangle = e^{-i E_m t/\hbar} | E_m(0) \rangle$$

TIME-DEPENDENCE OF THE STATIONARY STATES

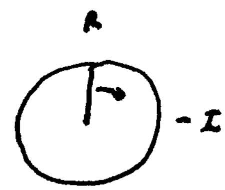
$$\psi_m(x,t) = e^{-i E_m t/\hbar}\, \psi_m(x)$$

IN POSITION SPACE

CLOCK HAND



$\omega_1 = E_1/\hbar$



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

$\omega_2 = 4\,\omega_1$

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

THE QUANTUM BABY RATTLE

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

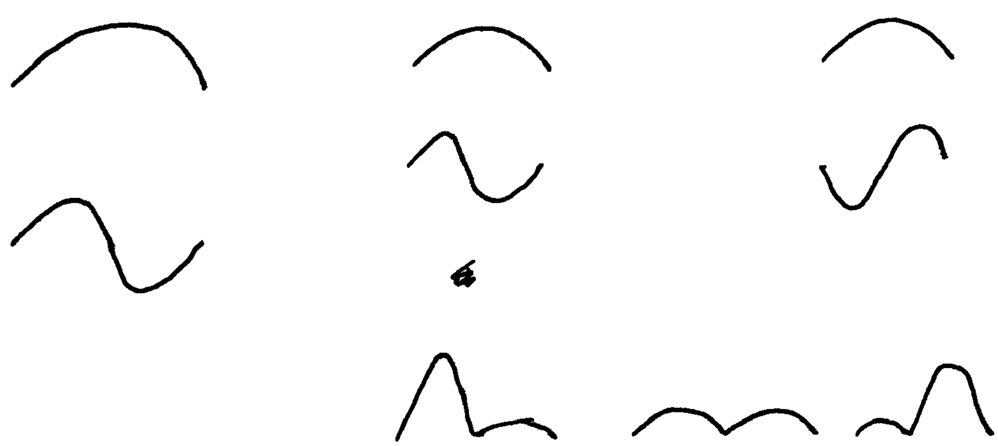
$$\psi(x,0) = \frac{1}{\sqrt{2}}\psi_1(x) + \frac{1}{\sqrt{2}}\psi_2(x)$$

TD

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}|E_1\rangle e^{-iE_1t/\hbar} + \frac{1}{\sqrt{2}}|E_2\rangle e^{-iE_2t/\hbar}$$

$$\psi(x,t) = \frac{1}{\sqrt{2}}\psi_1(x) e^{-iE_1t/\hbar} + \frac{1}{\sqrt{2}}\psi_2(x) e^{-iE_2t/\hbar}$$

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



50:50 SUPERPOSITION STATE

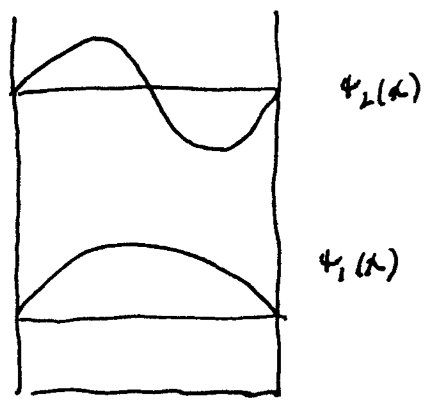
$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|E_1\rangle + \frac{1}{\sqrt{2}}|E_2\rangle$$

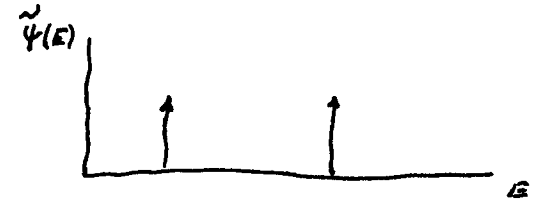
$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}|E_1\rangle e^{-iE_1t/\hbar} + \frac{1}{\sqrt{2}}|E_2\rangle e^{-iE_2t/\hbar}$$

$\langle x|$ $$\psi(x,t) = \frac{1}{\sqrt{2}}\psi_1(x)\, e^{-iE_1t/\hbar} + \frac{1}{\sqrt{2}}\psi_2(x)\, e^{-iE_2t/\hbar}$$

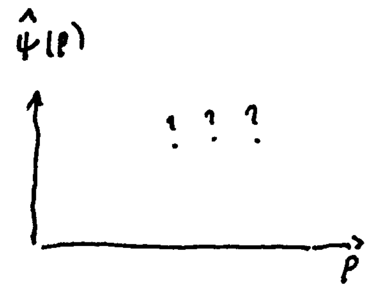
$\langle p|$ $$\hat{\psi}(p,t) = \frac{1}{\sqrt{2}}\hat{\psi}_1(p)\, e^{-iE_1t/\hbar} + \frac{1}{\sqrt{2}}\hat{\psi}_2(p)\, e^{-iE_2t/\hbar}$$

$\langle E|$ $$\tilde{\psi}(E,t) = \frac{1}{\sqrt{2}}\delta(E-E_1)\, e^{-iE_1t/\hbar} + \frac{1}{\sqrt{2}}\delta(E-E_2)\, e^{-iE_2t/\hbar}$$





TWO QUESTIONS:



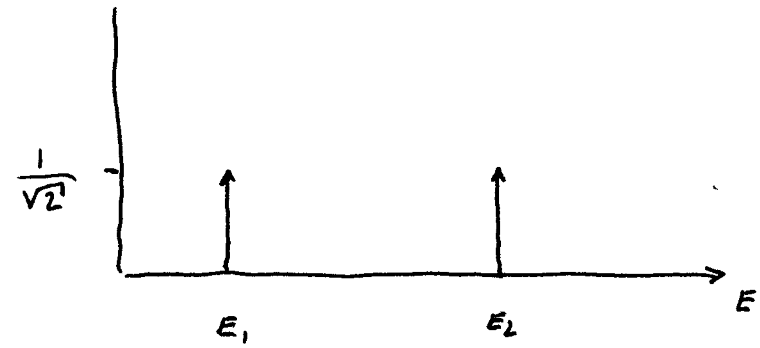
$\langle x(t)\rangle$

IF YOU MEASURE ....

ENERGY
POSSIBLE
RESULTS : EIGENVALUES OF THE HAMILTONIAN

EIGENENERGIES

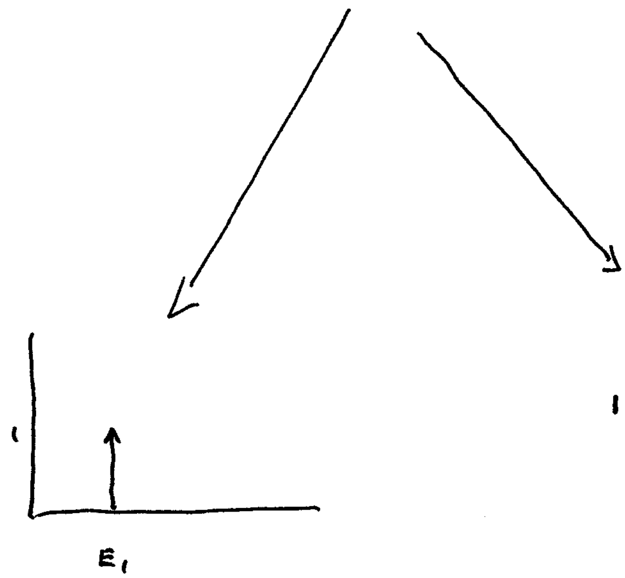
PROBABILITIES : HOW MUCH OF THAT EIGENSTATE IS IN $|\psi\rangle$

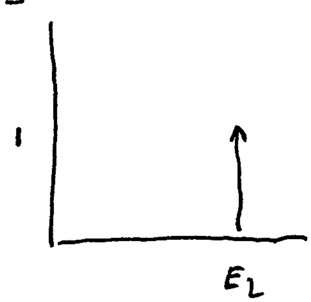


MYSTERIOUS QUANTUM JUMP

COLLAPSE OF THE WAVEFCN

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

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

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

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

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

FORMAL METHOD

MEASURE ENERGY

POSSIBILITIES : ev's OF H

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

PROB OF EACH ONE : 50% E_1 50% E_2

$$\text{PROB}(E_1) = \left| \langle E_1 | \Psi(t) \rangle \right|^2$$

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

$$= \left| \frac{1}{\sqrt{2}} e^{-iE_1 t/\hbar} \right|^2 = \frac{1}{2}$$

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

$$= \left| \frac{1}{\sqrt{2}} \frac{2}{a} \int_0^a \sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{\pi}{a} x\right) e^{-iE_1 t/\hbar} \, dx \right.$$

$$\left. + \frac{1}{\sqrt{2}} \frac{2}{a} \int_0^a \sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{2\pi}{a} x\right) e^{-iE_2 t/\hbar} \, dx \right|^2$$

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

WORKS FOR ANY $f(x) = \Psi(x,0)$

EXPECTATION VALUES

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

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

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

FOR THE QUANTUM RATTLE

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

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

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

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

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

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

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

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

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

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

$$= \frac{1}{2} E_1^2 + \frac{1}{2} E_2^2$$

since $E_2 = 4 E_1$

$$= \left(\frac{1}{2} + \frac{16}{2} \right) E_1^2$$

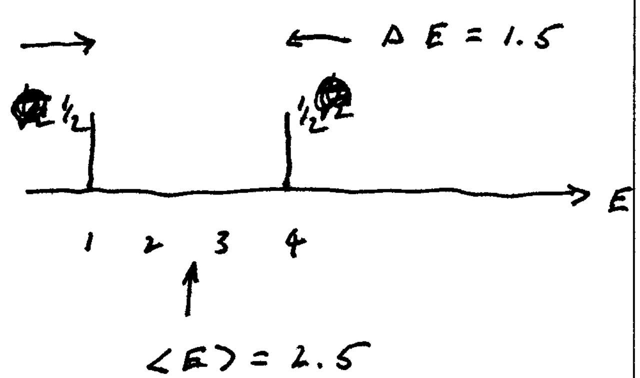
$$= \frac{17}{2} E_1^2 \qquad \text{TI}$$

$$\Delta H = \sqrt{\left(\langle H^2 \rangle - \langle H \rangle^2 \right)}$$

$$= \sqrt{\frac{17}{2} E_1^2 - \left(\frac{5}{2} E_1 \right)^2}$$

$$= \sqrt{\frac{34 - 25}{4} E_1^2} \qquad \text{TI}$$

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



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

$$\langle E_m | (xH - Hx) | E_m \rangle = \langle E_m | (-Hx + xH) | E_m \rangle$$

$$= \langle E_m | (-E_m x + x E_m) E_m \rangle$$

$$= 0$$

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

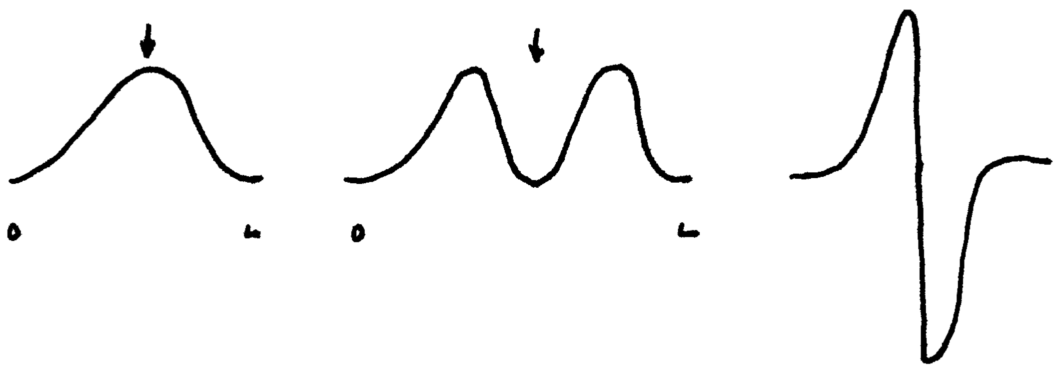
$$= \frac{1}{\sqrt{2}} \left(\langle E_1 | e^{+iE_1 t/\hbar} + \langle E_2 | e^{+iE_2 t/\hbar} \right) x$$

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

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

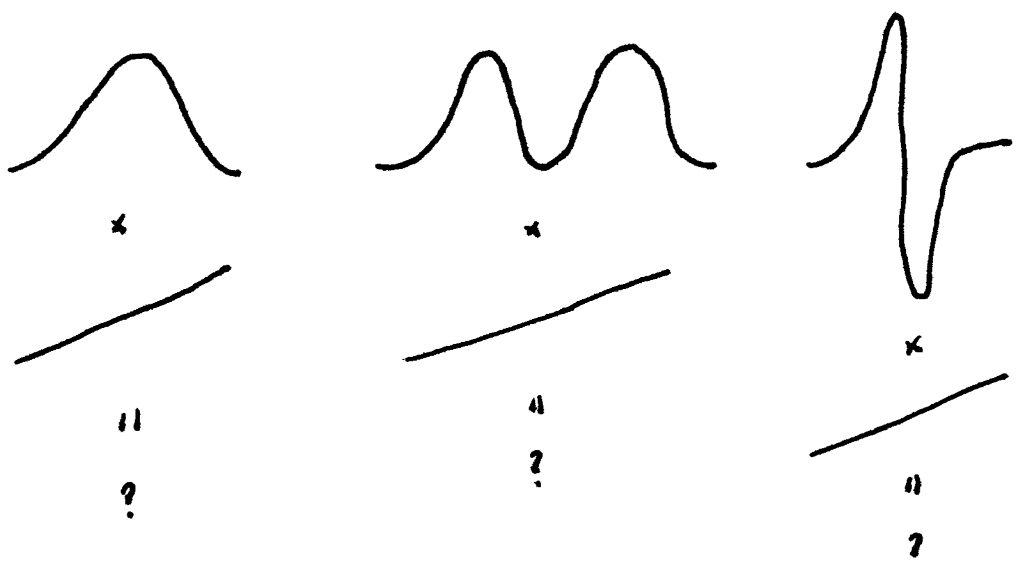
$$\langle x(t) \rangle = \int_0^L x \, dx \left[\frac{1}{2} \left| \psi_1(x) \right|^2 + \frac{1}{2} \left| \psi_2(x) \right|^2 + \psi_1(x) \, \psi_2(x) \cos(\Omega t) \right]$$

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

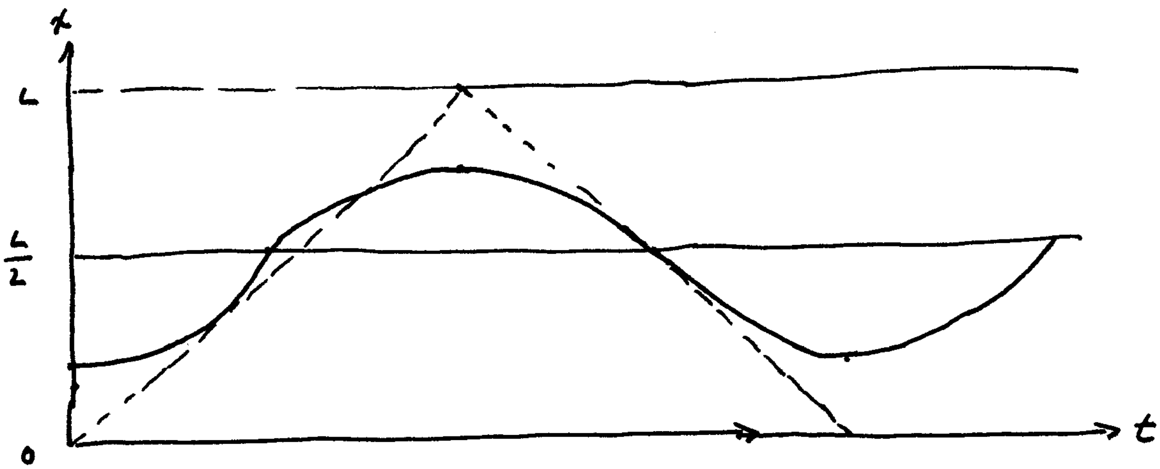


OSCILLATING

DOING THE INTEGRALS



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



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 $[p, H] = 0$

$$\langle E_n | pH - Hp | E_n \rangle$$

$$\langle E_n | -Hp + pH | E_n \rangle$$

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

$$0$$

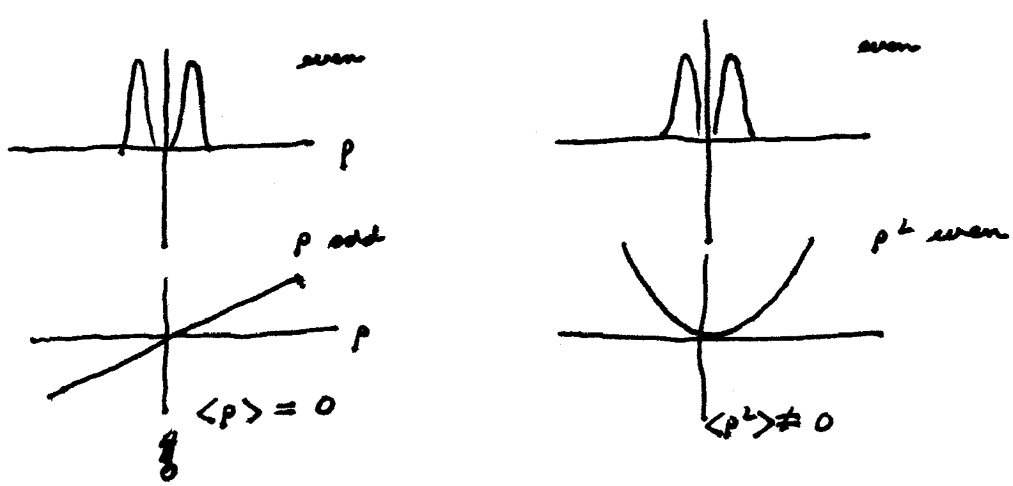
FOR THE ENERGY EIGENSTATES

$$\langle p \rangle = 0$$

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

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

FROM COMPUTER SIMULATION



QM BABY RATTLE

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

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

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

in x - space

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

in p - space

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

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

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

WAVEFUNCTIONS IN MOMENTUM SPACE

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

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

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

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

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

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

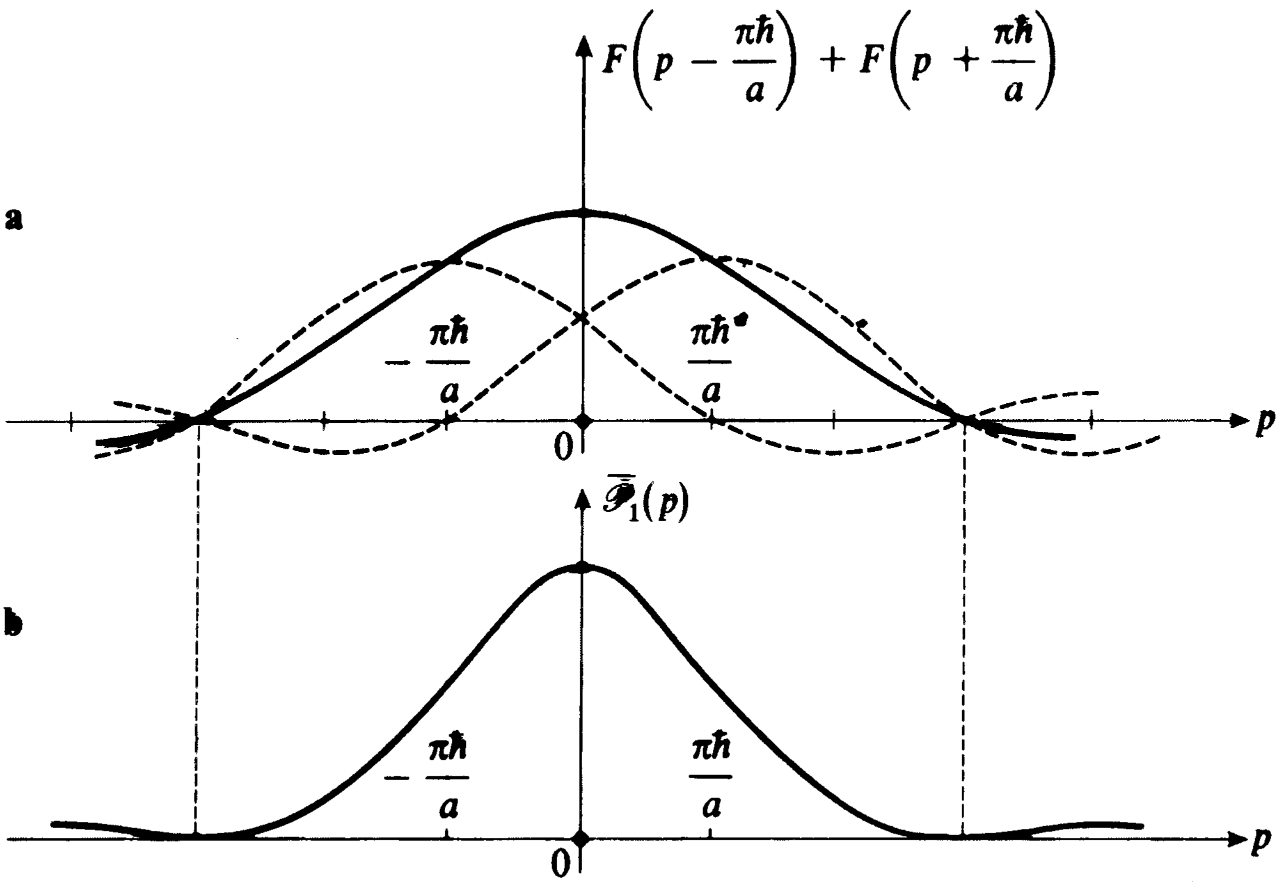
$$\hat{\psi}_n(p) = \frac{1}{2i}\sqrt{\frac{a}{\pi\hbar}}\; e^{i\left(\frac{n\pi}{2} - \frac{pa}{2\hbar}\right)}$$

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

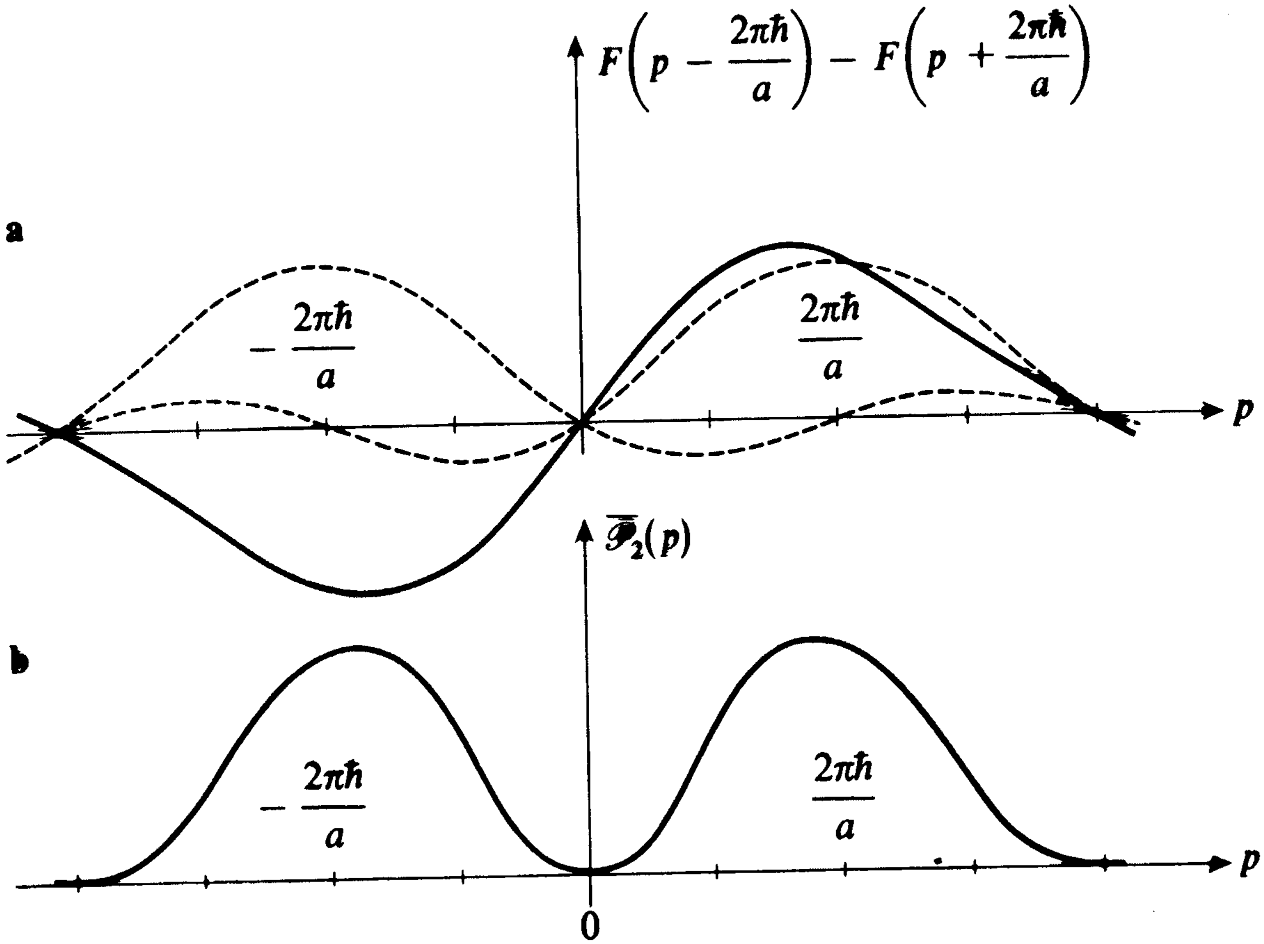
$$F(p) = \frac{\sin(pa/2\hbar)}{(pa/2\hbar)}$$

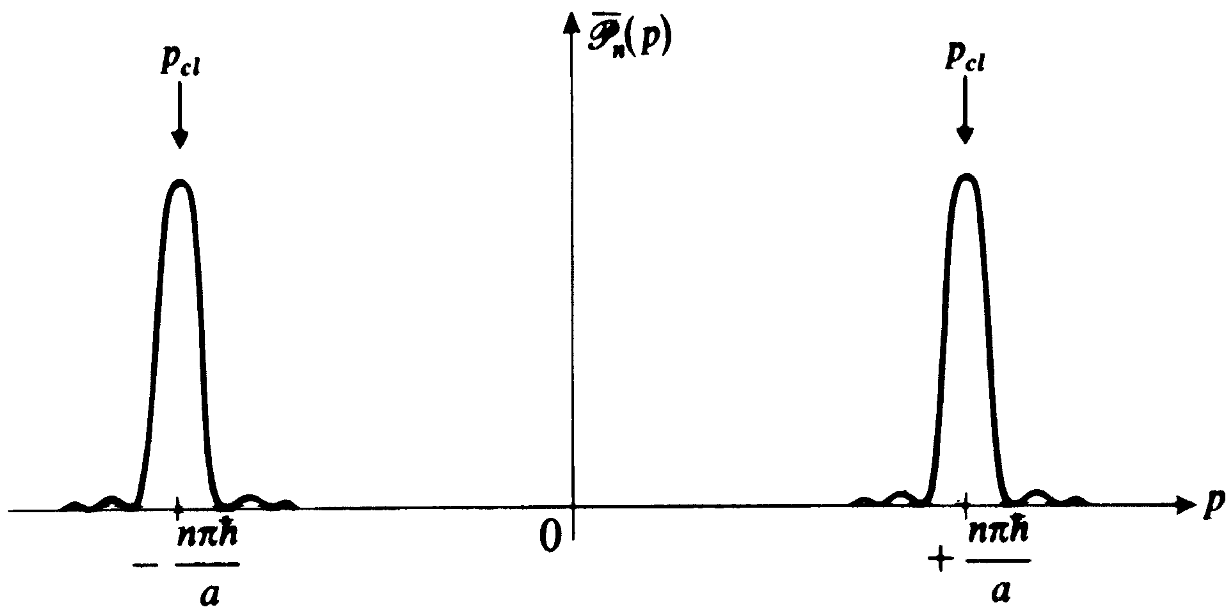
$$= \frac{\sin x}{x}$$

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

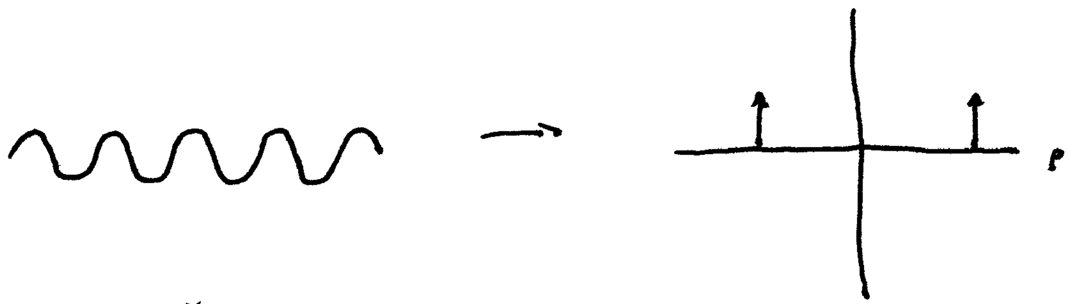


$F\left(p - \frac{\pi\hbar}{a}\right) + F\left(p + \frac{\pi\hbar}{a}\right)$
a
$-\frac{\pi\hbar}{a}$
$\frac{\pi\hbar}{a}$
0
p
$\bar{\mathscr{P}}_1(p)$
b
$-\frac{\pi\hbar}{a}$
$\frac{\pi\hbar}{a}$
0
p

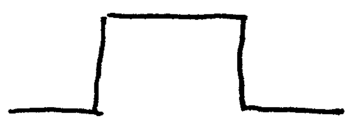

$F\left(p - \frac{2\pi\hbar}{a}\right) - F\left(p + \frac{2\pi\hbar}{a}\right)$
a
$-\frac{2\pi\hbar}{a}$
$\frac{2\pi\hbar}{a}$
p
$\bar{\mathcal{P}}_2(p)$
b
$-\frac{2\pi\hbar}{a}$
$\frac{2\pi\hbar}{a}$
p
0

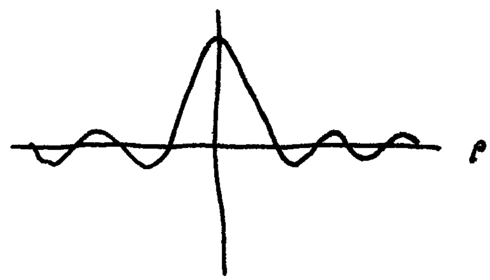

p_{cl}
$\overline{\mathscr{P}}_n(p)$
p_{cl}
p
$-\frac{n\pi\hbar}{a}$
0
$+\frac{n\pi\hbar}{a}$

CARTOON VERSION

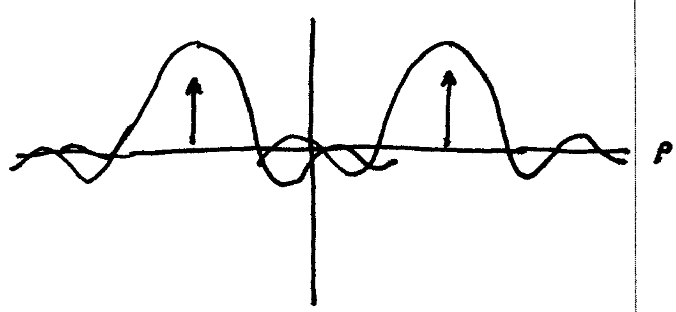


$\times$ $\qquad\qquad\qquad\qquad$ $\otimes$



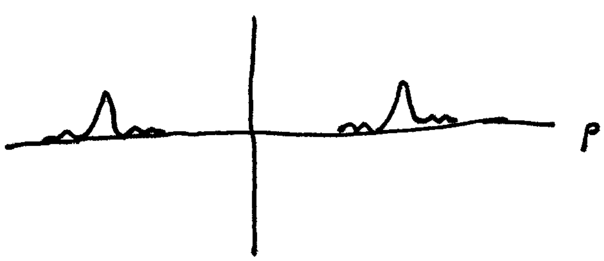


$=$

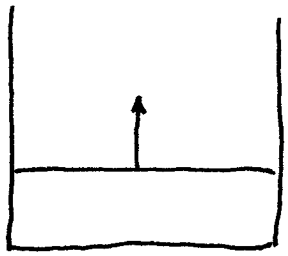


$$\boxed{\begin{array}{c} A \cdot B = C \iff \hat{A} \otimes \hat{B} = \hat{C} \\ \text{CONVOLUTION THEOREM} \end{array}}$$

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



MEASURE x FIND IN CENTER OF WELL



BY SYMMETRY => ONLY ODD n

yes

yes

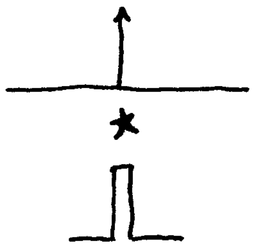
no

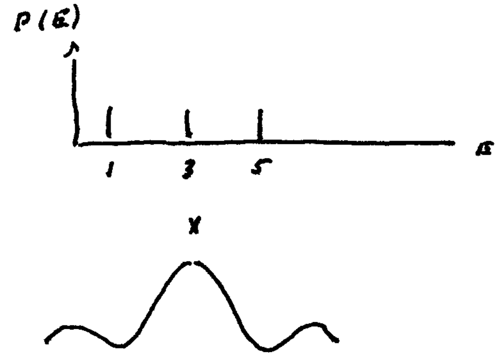
$$P(E_n) = \frac{2}{a} \quad n \text{ odd}$$

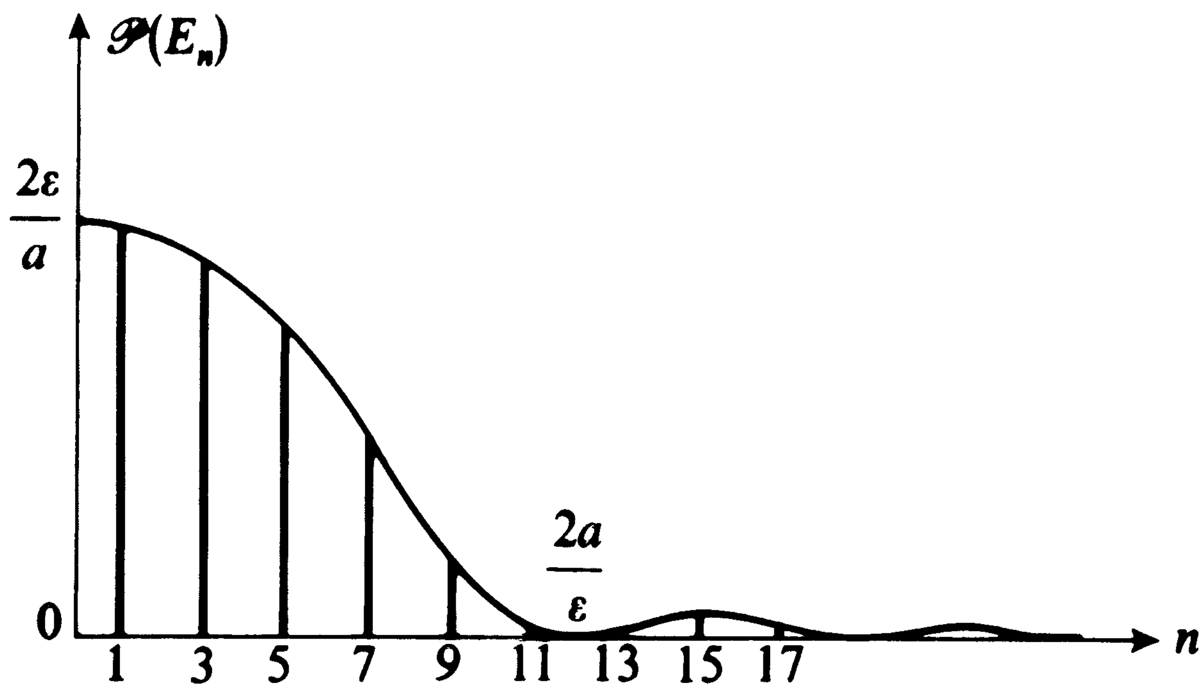
$$= 0 \quad n \text{ even}$$

=> ∞ ENERGY

FINITE X RESOLUTION







$\mathscr{P}(E_n)$
$\frac{2\varepsilon}{a}$
$\frac{2a}{\varepsilon}$
0
1
3
5
7
9
11
13
15
17
n