Step-by-step procedure to solve QM problems

(1) Solve the TISE

$$H\,|E_n>=E_n\,|E_n>$$

Diagonalize the Hamiltonian
Find the eigenvalues E_n
Find the eigenstates $|E_n>$

(2) Expand $|\psi(0)>$ in energy eigenstates

$$|\psi(0)>=\sum_n a_n\,|E_n>$$

The energy eigenstates are called stationary states

(3) Put in the time-dependent phase factors $e^{(-iE_nt/\hbar)}$

$$|\psi(t)>=\sum_n a_n\,e^{(-iE_nt/\hbar)}\,|E_n>$$

$\boxed{\textbf{Expand } |\psi(0)> \textbf{ in the energy basis}}$

$$|\psi(0)> = |E_1> + |E_2> + |E_3>$$

$$|\psi(0)> = I\ |\psi(0)>$$

$$I = \sum_n |E_n><E_n|$$

$$|\psi(0)> = \sum_n |E_n><E_n|\psi(0)>$$

$$a_n = <E_n|\psi(0)>$$

$$|\psi(0)> = \sum_n |E_n> a_n = \sum_n a_n\ |E_n>$$

Write down $|\psi(t)>$ by inspection in energy basis

$$|\psi(t)> = \sum_{all\ n} a_n\ |E_n> exp(-iE_n t/\hbar)$$

$$\psi(x,t) = \sum_{all\ n} a_n\ \psi_n(x)\ exp(-iE_n t/\hbar)$$

Just insert the time-dependent phase factors

Warning: This only works in the energy basis!!!

Eigenvector Example

In Dirac notation

$$|\psi(0)>= N\ (|E_1> + |E_2> + |E_3>)$$

In vector notation

$$\psi(0) = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

In Dirac notation

$$|\psi(t)>= \frac{1}{\sqrt{3}} \left(e^{-iE_1 t/\hbar}|E_1> + e^{-iE_2 t/\hbar}|E_2> + e^{-iE_3 t/\hbar}|E_3> \right)$$

In vector notation

$$\psi(t) = \frac{1}{\sqrt{3}}\ e^{-iE_1 t/\hbar} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{3}}\ e^{-iE_2 t/\hbar} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{3}}\ e^{-iE_3 t/\hbar} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\psi(t) = \frac{1}{\sqrt{3}} \begin{pmatrix} e^{-iE_1 t/\hbar} \\ e^{-iE_2 t/\hbar} \\ e^{-iE_3 t/\hbar} \end{pmatrix}$$

Eigenfunction Example

In Dirac notation

$$|\psi(0)>= N\left(|E_1> + |E_2> + |E_3>\right)$$

In eigenfunction notation

$$\psi(x,0) = N\Big(\psi_1(x) + \psi_2(x) + \psi_3(x)\Big)$$

In Dirac notation

$$|\psi(t)>= \frac{1}{\sqrt{3}}\left(e^{-iE_1t/\hbar}|E_1> + e^{-iE_2t/\hbar}|E_2> + e^{-iE_3t/\hbar}|E_3>\right)$$

In eigenfunction notation

$$\psi(x,t) = \frac{1}{\sqrt{3}}\left(\psi_1(x)e^{-iE_1t/\hbar} + \psi_2(x)e^{-iE_2t/\hbar} + \psi_3(x)e^{-iE_3t/\hbar}\right)$$

The $\psi_n(x)$ functions are called the eigenfunctions or the stationary states, and they are given by

$$\psi_1(x) = < x\,|E_1>$$
$$\psi_2(x) = < x\,|E_2>$$
$$\psi_3(x) = < x\,|E_3>$$

Possibilities and Probabilities

In Dirac notation

$$|\psi(0)>= N\ (|E_1> + |E_2> + |E_3>)$$

If you measure the energy, what are the possibilities and what are the corresponding probabilities?

The possibilities are the eigenvalues of the Hamiltonian.

So, the possibilities are E_1, E_2, E_3.

The probabilities are given by $| < E_i \mid \psi > |^2$.

So, the probabilities are $\frac{1}{3}$, $\frac{1}{3}$, $\frac{1}{3}$.

What is the state of the system immediately after the measurement?

The state is in the eigenstate of H corresponding to the measured eigenvalue.

So, the state is $|E_1>$ or $|E_2>$ or $|E_3>$.

For the eigenvector example

$$|E_1 >=> \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$|E_2 >=> \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$|E_3 >=> \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

For the eigenfunction example

$$\psi_1(x) = < x \mid E_1 >$$
$$\psi_2(x) = < x \mid E_2 >$$
$$\psi_3(x) = < x \mid E_3 >$$

$\boxed{\text{To find the } a_n \text{ expansion coefficients}}$

$$|\psi(0)>=\sum_n a_n\,|E_n>$$

Compute the inner products

$$a_n = <E_n|\psi(0)>$$

In the vector example

$$a_1 = <E_1|\psi(0)>=(1,0,0)\,\frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix} = \frac{1}{\sqrt{3}}$$

$$a_2 = <E_2|\psi(0)>=(0,1,0)\,\frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix} = \frac{1}{\sqrt{3}}$$

$$a_3 = <E_3|\psi(0)>=(0,0,1)\,\frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix} = \frac{1}{\sqrt{3}}$$

In the eigenfunction example

$$a_1 = <E_1|\psi(0)>$$

$$a_2 = <E_2|\psi(0)>$$

$$a_3 = <E_3|\psi(0)>$$

Still compute the inner products, but ....

Still compute the inner products, but the inner products are now given by integrals

$$a_1 = < E_1|\psi(0) >= \int \psi_1^*(x)\, \psi(x,0)\, dx$$

$$a_2 = < E_2|\psi(0) >= \int \psi_2^*(x)\, \psi(x,0)\, dx$$

$$a_3 = < E_3|\psi(0) >= \int \psi_3^*(x)\, \psi(x,0)\, dx$$

Note that the probabilities are given by the magnitude squared of the expansion coefficients $Prob(E_n) = |a_n|^2$

$$Prob(E_1) = |a_1|^2 = |< E_1|\psi(0) >|^2 = \left| \int \psi_1^*(x)\, \psi(x,0)\, dx \right|^2$$

$$Prob(E_2) = |a_2|^2 = |< E_2|\psi(0) >|^2 = \left| \int \psi_2^*(x)\, \psi(x,0)\, dx \right|^2$$

$$Prob(E_3) = |a_3|^2 = |< E_3|\psi(0) >|^2 = \left| \int \psi_3^*(x)\, \psi(x,0)\, dx \right|^2$$

$\boxed{\text{The Square Well aka The Particle in a Box}}$

Time-Independent Schrodinger Equation (TISE)

$$H\ |E_n >= E_n\ |E_n >$$

In position space

$$H_{op}\ \psi_n(x) = E_n \psi_n(x)$$

$$H_{op} = \frac{p_{op}^2}{2m} + V(x_{op})$$

$$p_{op} = -i\hbar \frac{d}{dx}$$

$$x_{op} = x$$

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

For the square well

$$V(x) = 0$$

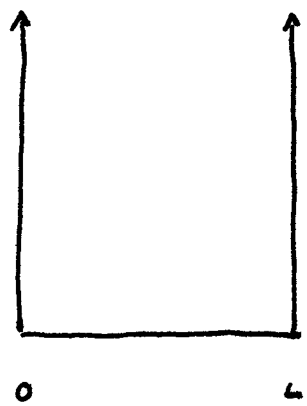
So TISE becomes this differential equation

$$H\ \psi_n(x) = \frac{-\hbar^2}{2m}\ \frac{d^2}{dx^2}\ \psi_n(x) = E_n\ \psi_n(x)$$

LECTURE 13 JULY 13, 2007

INFINITE SQUARE WELL

"PARTICLE IN A BOX"



SOLVE TISE $\Rightarrow$ STATIONARY STATES (TI)

$\Downarrow$

TIME-DEPENDENT STATES

Expand t=0 the wavefunction and insert the phase factors

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

The TISE

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

The differential equation

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

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

GENERAL SOLUTION

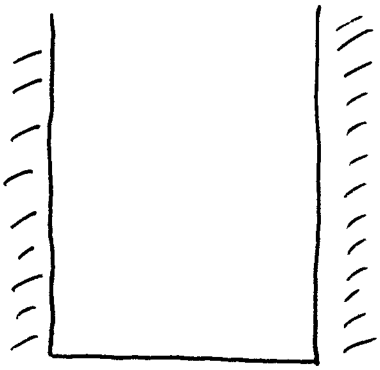
$$\cancel{K=}\sqrt{2mE/\hbar^2} = K$$

WE NEED TO FIND ef's OF H

en's OF H

SQUARE WELL

aka, PARTICLE IN A BOX



INSIDE

$V(x) = 0$

AT BOUNDARY AND

OUTSIDE $V(x) = \infty$

$\Rightarrow$ PARTICLE

CANNOT

GET OUTSIDE

even if only walls

$= \infty$, particle cannot

escape

TISE $\quad H\psi = E\psi$

$$\cancel{H\psi} \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \cancelto{0}{V(x)} \right] \psi_n(x) = E_n \psi_n(x)$$

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_n(x) = E_n \psi_n(x)$$

FIND THESE FCN S

ef's

AND THESE NUMBERS

en's

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

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

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

$$A \sin(k_n x)$$

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

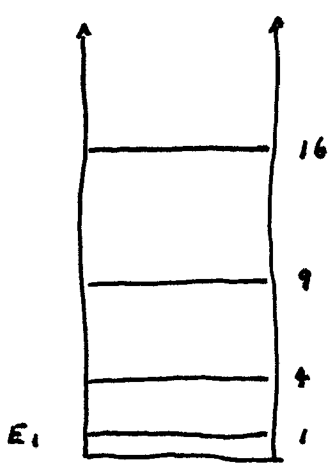
NORMALIZED STATIONARY STATES

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

eigenfunctions

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

eigenenergies



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

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.

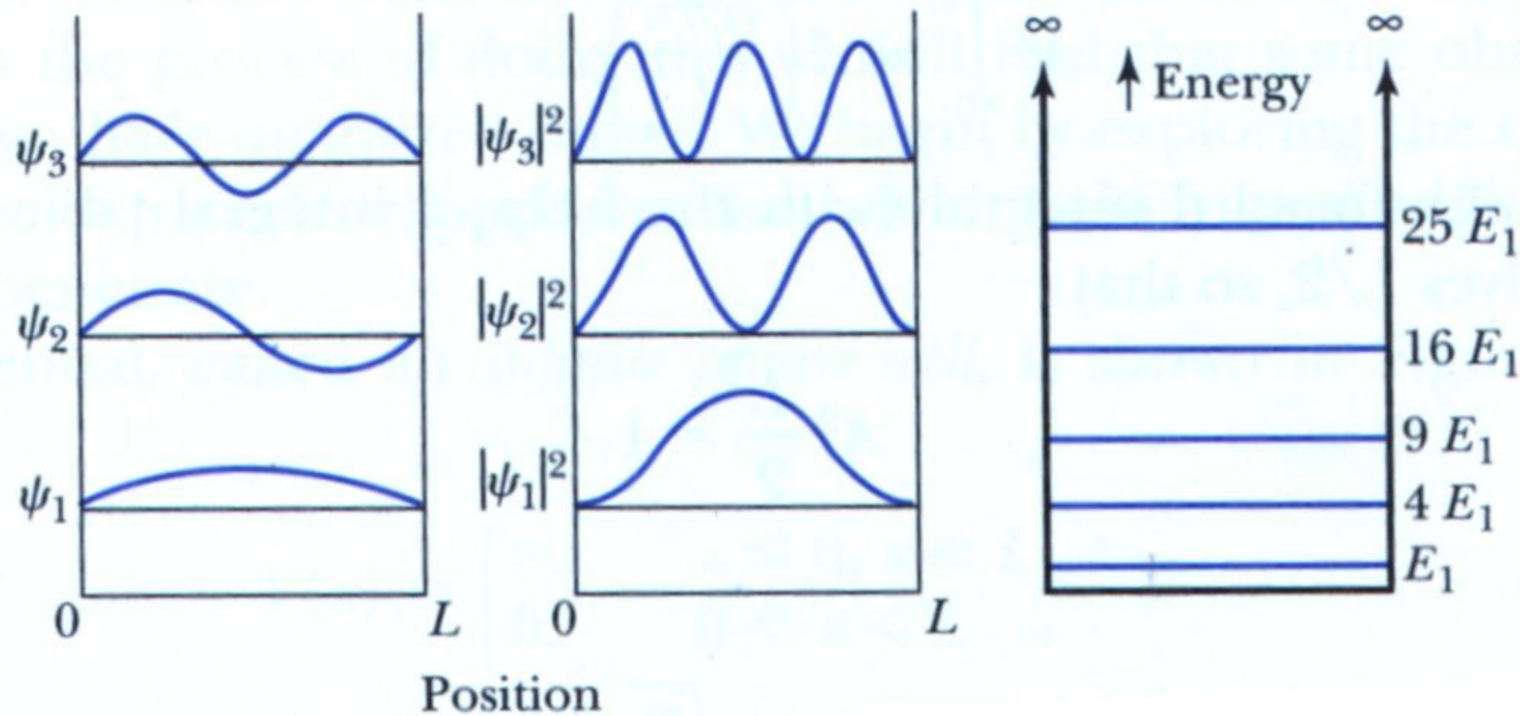
The Square Well

The Particle in a Box

wavefunctions

probability densities

eigenenergies



Measure the position: The probability to find the particle precisely at x=2 is zero. But the probability to find the particle at x=2 plus/minus 0.01 is non-zero.

http://en.wikipedia.org/wiki/Particle_in_a_box

The Square Well

http://www.falstad.com/qm1d

http://phet.colorado.edu/en/simulation/bound-states

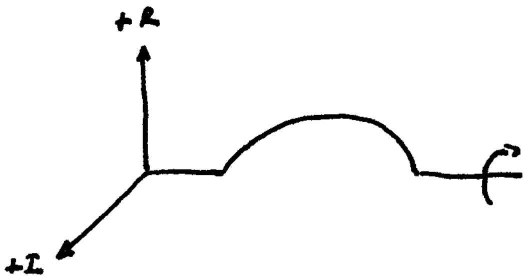
TIME-DEPENDENCE OF THE ENERGY EIGENKETS

$$|E_n(t)\rangle = e^{-iE_nt/\hbar}\,|E_n(0)\rangle$$

TIME-DEPENDENCE OF THE STATIONARY STATES

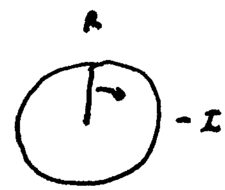
$$\psi_n(x,t) = e^{-iE_nt/\hbar}\,\psi_n(x)$$

IN POSITION SPACE



$\omega_1 = E_1/\hbar$

CLOCK HAND



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

$\omega_2 = 4\omega_1$

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

TIME - DEPENDENCE

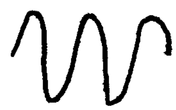
$$\psi(x,t) = a_1 e^{-i\omega_1 t}$$

T_1

$$+ a_3 e^{-i\omega_3 t}$$

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

$$+ a_5 e^{-i\omega_5 t}$$



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

$$\boxed{\Rightarrow \text{RECURRENCE TIME} = T_1 \,!}$$

EXPANSION IN DIFFERENT SPACES / BASES

E, x, p

energy E

position x

momentum p

SUPERPOSITION OF 3 LOWEST STATES

PROB $\frac{1}{3}$ $\frac{1}{3}$ $\frac{1}{3}$

In Dirac notation: the abstract state vector in Hilbert space

$$|\psi\rangle = \frac{1}{\sqrt{3}}|E_1\rangle + \frac{1}{\sqrt{3}}|E_2\rangle + \frac{1}{\sqrt{3}}|E_3\rangle \quad \text{ABSTRACT}$$

In the position basis, aka in position space

$$\langle x|\psi\rangle = \frac{1}{\sqrt{3}}\langle x|E_1\rangle + \frac{1}{\sqrt{3}}\langle x|E_2\rangle + \frac{1}{\sqrt{3}}\langle x|E_3\rangle$$

$$\psi(x) = \frac{1}{\sqrt{3}}\psi_1(x) + \frac{1}{\sqrt{3}}\psi_2(x) + \frac{1}{\sqrt{3}}\psi_3(x)$$

In the momentum basis, aka in momentum space

$$\langle p|\psi\rangle = \frac{1}{\sqrt{3}}\langle p|E_1\rangle + \frac{1}{\sqrt{3}}\langle p|E_2\rangle + \frac{1}{\sqrt{3}}\langle p|E_3\rangle$$

$$\hat{\psi}(p) = \frac{1}{\sqrt{3}}\hat{\psi}_1(p) + \frac{1}{\sqrt{3}}\hat{\psi}_2(p) + \frac{1}{\sqrt{3}}\hat{\psi}_3(p)$$

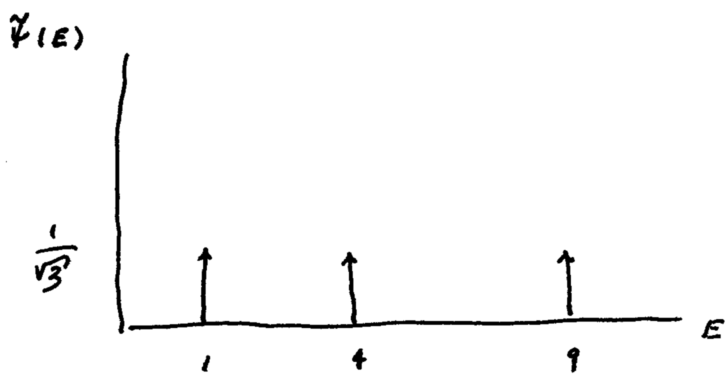
HOW ABOUT $\psi(E)$?

In the energy basis, aka in energy space

$$\langle E|\psi\rangle \cancel{\psi(E)} = \frac{1}{\sqrt{3}}\langle E|E_1\rangle + \frac{1}{\sqrt{3}}\langle E|E_2\rangle + \frac{1}{\sqrt{3}}\langle E|E_3\rangle$$

$$\tilde{\psi}(E) = \frac{1}{\sqrt{3}}\tilde{\psi}_1(E) + \frac{1}{\sqrt{3}}\tilde{\psi}_2(E) + \frac{1}{\sqrt{3}}\tilde{\psi}_3(E)$$

$$= \frac{1}{\sqrt{3}}\delta(E-E_1) + \frac{1}{\sqrt{3}}\delta(E-E_2) + \frac{1}{\sqrt{3}}\delta(E-E_3)$$



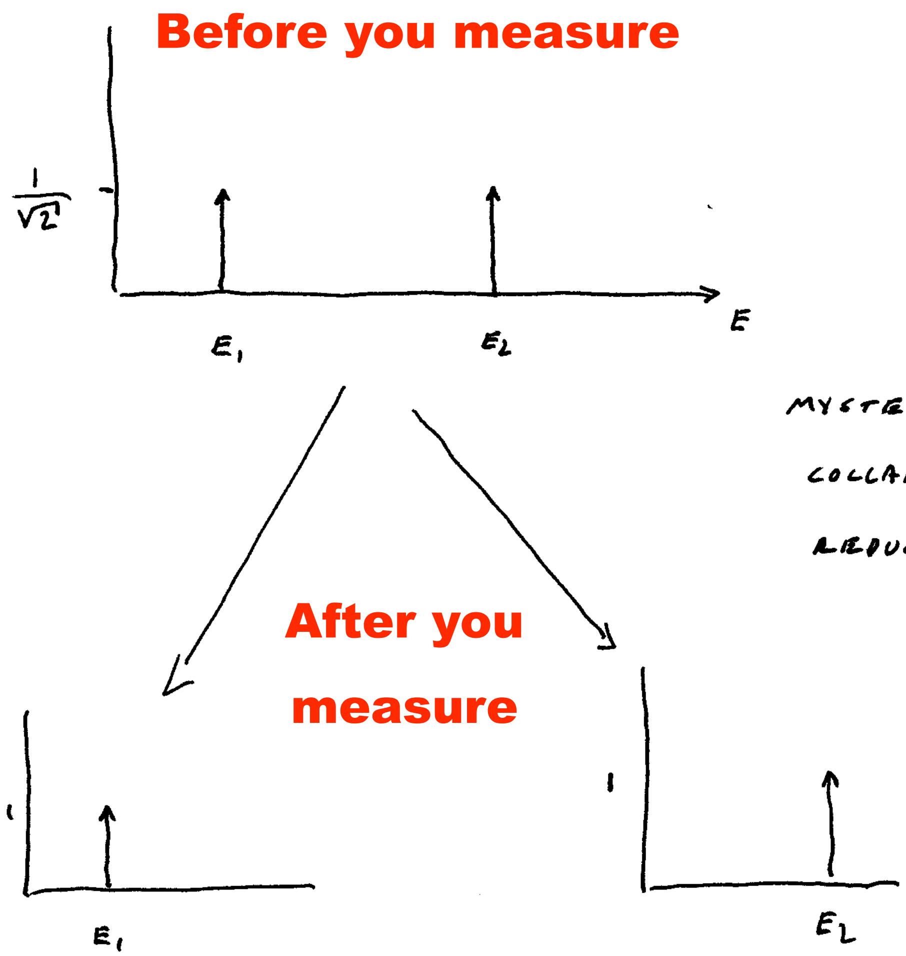
IF YOU MEASURE ....

Measure the Energy

ENERGY POSSIBLE RESULTS : EIGENVALUES OF THE HAMILTONIAN

EIGENENERGIES

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



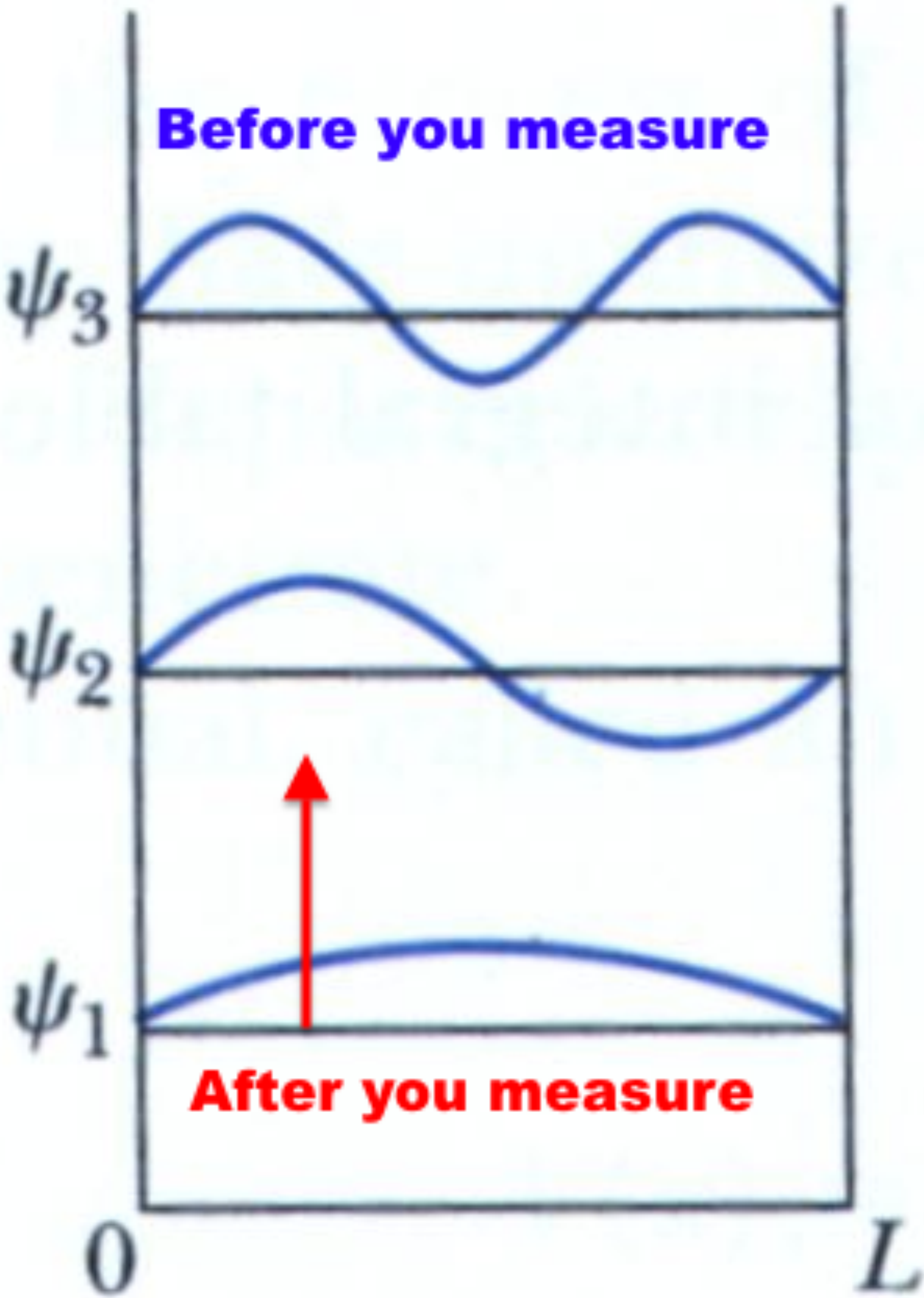
MYSTERIOUS QUANTUM JUMP

COLLAPSE OF THE WAVEFCN

REDUCTION OF THE STATE VECTOR

MYSTERIOUS BECAUSE :

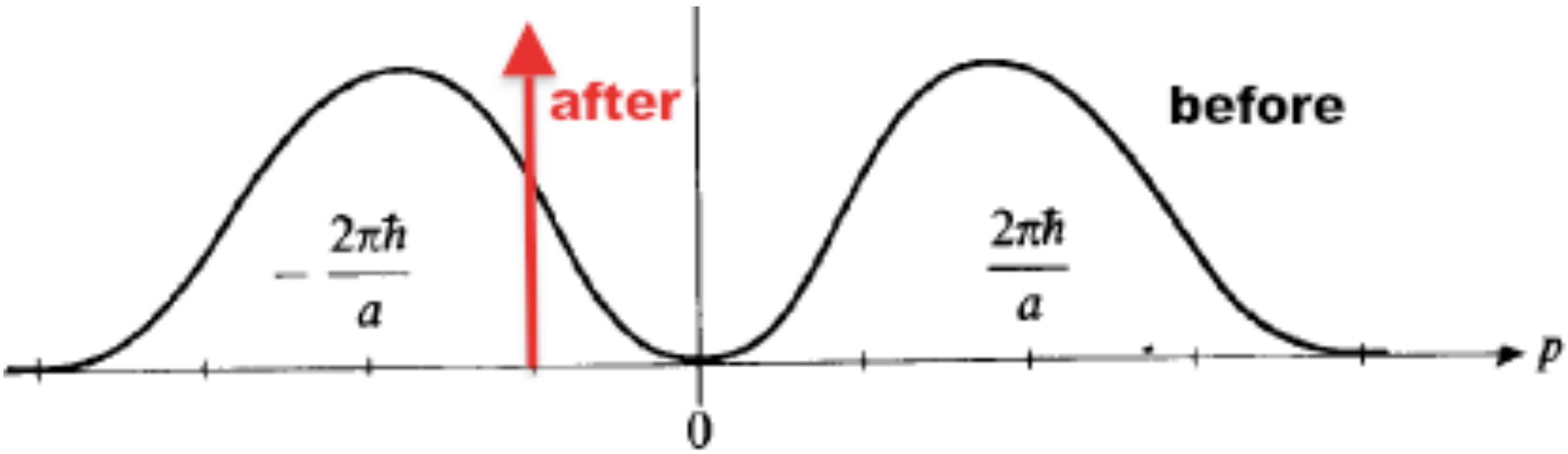
Measure the Position

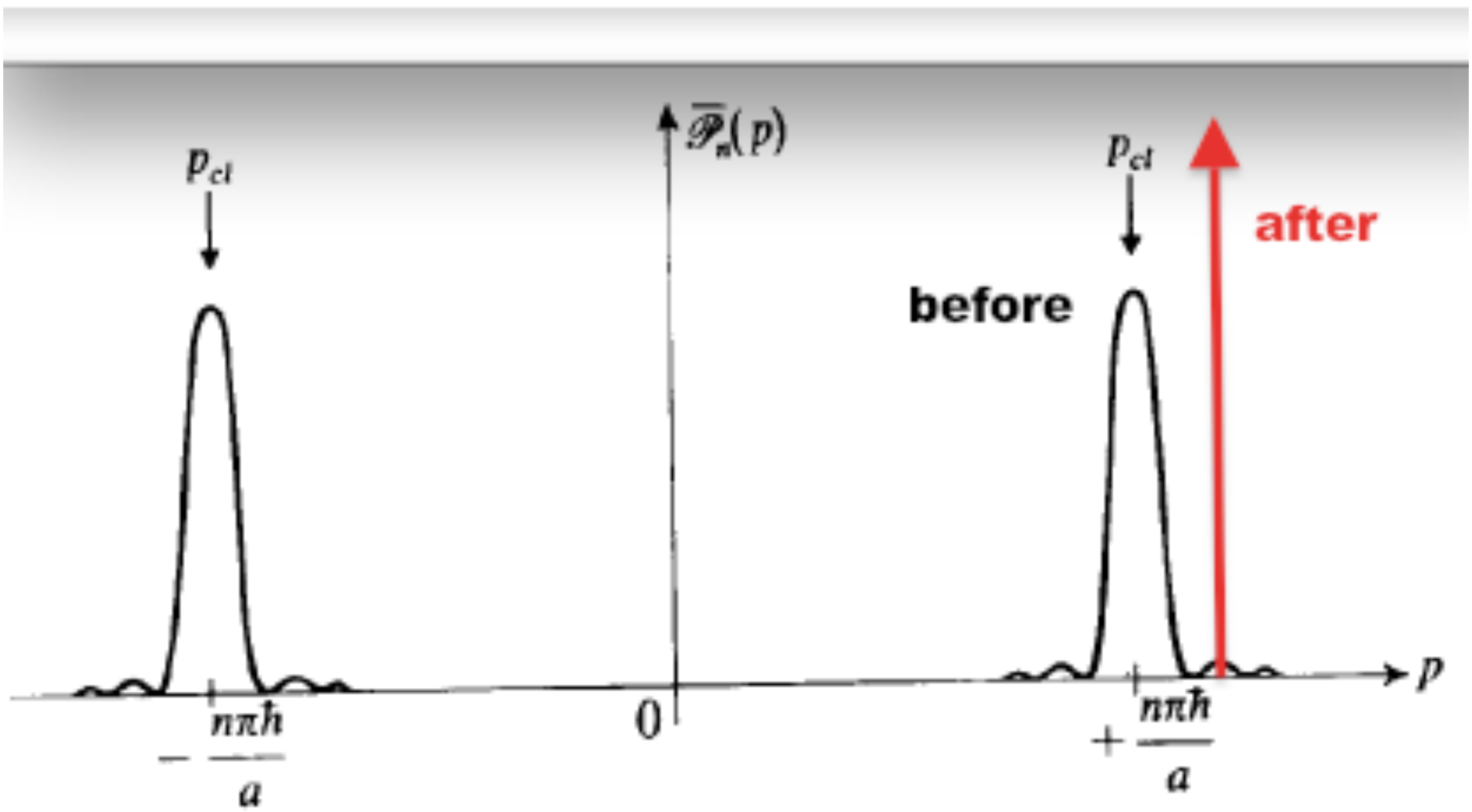


If you measure the momentum

when n=2

probability density in momentum-space





when n is large

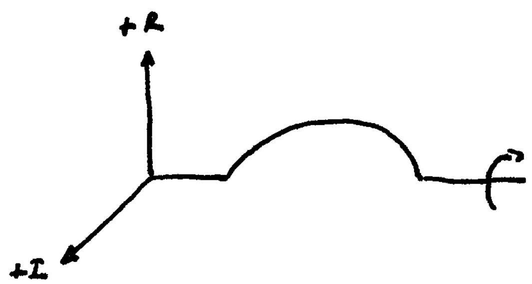
TIME-DEPENDENCE OF THE ENERGY EIGENKETS

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

TIME-DEPENDENCE OF THE STATIONARY STATES

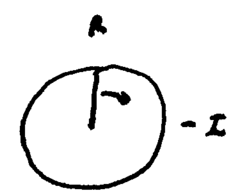
$$\psi_n(x,t) = e^{-iE_nt/\hbar} \psi_n(x)$$

IN POSITION SPACE



$\omega_1 = E_1/\hbar$

CLOCK HAND



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

$\omega_2 = 4\omega_1$

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