February 13, 2012

Finish Free Particle

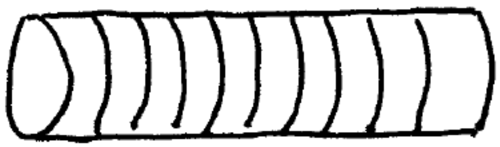
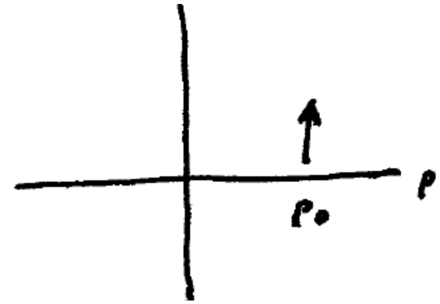
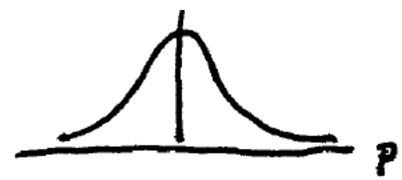
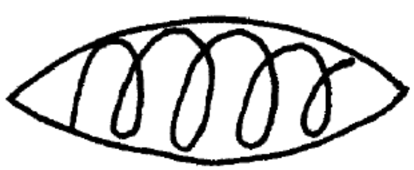
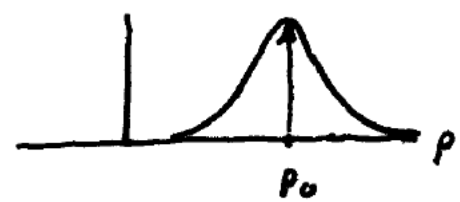
(1) Qualitative

(2) Quantitative

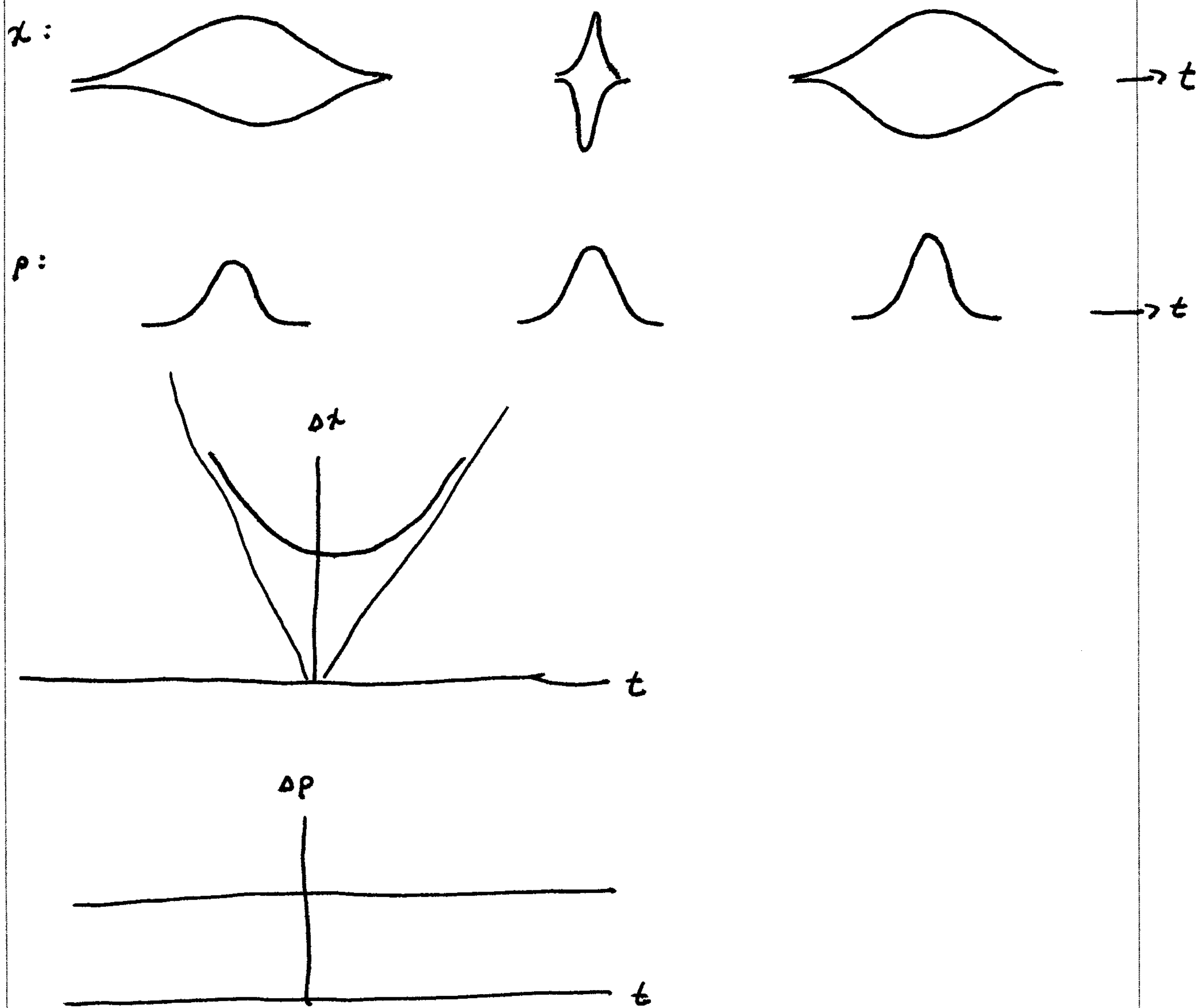
Start Simple Harmonic Oscillator

(1) Solve Differential Equation (today)

(2) Use the Algebra of the Operators

position space		momentum space
A plane wave	<=>	A delta function at $p=p_o$
	<=>	
times	<=>	convolved with
A Gaussian	<=>	A Gaussian at $p=0$
	<=>	
is equal to	<=>	is equal to
A wavepacket	<=>	A Gaussian at $p=p_o$
	<=>	

Cartoon Version of the Free Particle



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http://www.st-andrews.ac.uk/~qmanim/embed_item_3.php?anim_id=1

http://www.physics.nus.edu.sg/einstein/lect14/applets/propa.html

http://www.brainflux.org/java/classes/Schrodinger1D.html

http://demonstrations.wolfram.com/WavepacketForAFreeParticle/

http://demonstrations.wolfram.com/EvolutionOfAGaussianWavePacket/

Quantitative Evolution

(1) FINISH FREE WAVE PACKET

QUANTITATIVE

(2) START HARMONIC OSCILLATOR

$$\psi(x,0) = e^{ip_0 x/\hbar} \quad (\pi^{\circ}\Delta^2)^{-1/4} \quad e^{-x^2/2\Delta^2}$$

PLANE WAVE

GAUSSIAN ENVELOPE

$\langle p \rangle = p_0$

$\Delta p = \dfrac{\hbar}{\sqrt{2}\,\Delta}$

$\langle x \rangle = 0$

$\Delta x = \dfrac{\Delta}{\sqrt{2}}$

$$\Delta x \, \Delta p = \frac{\hbar}{2}$$

MINIMUM UNCERTAINTY AT $t = 0$

INCLUDE THE TIME-DEPENDENT PHASE FACTORS

$$e^{-iE_m t/\hbar} = e^{-i(p^2/2m)t/\hbar}$$

PROPAGATOR $\quad U(x,t;x',t') = \sqrt{m/2\hbar i(t-t')}\; e^{-im(x-x')/2\hbar(t-t')}$

$\cancel{\psi(x,t) = \int U(x,t)\,\psi(}$

$$\boxed{\begin{aligned} U(t) &= \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-iE(p)t/\hbar} \\ &= \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-i(p^2/2m)t/\hbar} \end{aligned}}$$

propagator in Hilbert space

STILL IN THE HILBERT SPACE

IN X-SPACE

$$\langle x | U(t) | x' \rangle = \int \langle x | p \rangle \langle p | x' \rangle\, e^{-ip^2t/2m\hbar}\, dp$$

$$= \int e^{ip(x-x')/\hbar}\, e^{-ip^2t/2m\hbar}\, dp$$

$$\boxed{\begin{aligned} &= \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x')/2\hbar t} \\ &= U(x, t; x', 0) \\ &= U(x, t; x', t') \qquad t \to t - t' \end{aligned}}$$

propagator in position space

$\langle \omega | U(t) | \omega' \rangle$ MATRIX ELEMENTS

$$\nabla^2 T = \kappa \frac{\partial T}{\partial t}$$ **heat equation**

$$\nabla^2 \psi = \gamma \frac{d\psi}{d(it)}$$ **TDSE is the heat eqn in imaginary time**

the wavepacket spreads like heat spreads => like a Gaussian

Non-relativistic propagators [edit]

In non-relativistic quantum mechanics the propagator gives the amplitude for a particle to travel from one spatial point at one time to another spatial point at a later time. It is a Green's function for the Schrödinger equation. This means that if a system has Hamiltonian H then the appropriate propagator is a function $K(x,t;x',t')$ satisfying

$$\left(H_x - i\hbar\frac{\partial}{\partial t}\right) K(x,t;x',t') = -i\hbar\delta(x-x')\delta(t-t')$$

where H_x denotes the Hamiltonian written in terms of the x coordinates and $\delta(x)$ denotes the Dirac delta-function.

This can also be written as

$$K(x,t;x',t') = \langle x|\hat{U}(t,t')|x'\rangle$$

where $\hat{U}(t,t')$ is the unitary[disambiguation needed] time-evolution operator for the system taking states at time t to states at time t'.

Path integral in quantum mechanics [edit]

The quantum mechanical propagator may also be found by using a path integral.

$$K(x,t;x',t') = \int \exp\left[\frac{i}{\hbar}\int_t^{t'} L(\dot{q},q,t)dt\right] D[q(t)]$$

where the boundary conditions of the path integral include q(t)=x, q(t')=x'. Here L denotes the Lagrangian of the system. The paths that are summed over move only forwards in time.

Using the quantum mechanical propagator [edit]

In non-relativistic quantum mechanics, the propagator lets you find the state of a system given an initial state and a time interval. The new state is given by the equation:

$$\psi(x,t) = \int_{-\infty}^{\infty} \psi(x',t') K(x,t;x',t') dx'.$$

If $K(x,t;x',t')$ only depends on the difference $x - x'$ this is a convolution of the initial state and the propagator.

Propagator of Free Particle and Harmonic Oscillator [edit]

For time translational invariant system, the propagator only depends on the time difference (t-t'), thus it may be rewritten as

$$K(x,t;x',t') = K(x,x';t-t').$$

The propagator of one-dimensional free particle, with the far-right expression obtained via saddle-point approximation[1], is then

$$K(x,x';t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \, e^{ik(x-x')} e^{-i\hbar k^2 t/(2m)} = \left(\frac{m}{2\pi i\hbar t} \right)^{1/2} e^{-m(x-x')^2/(2i\hbar t)}$$

.

The propagator of one-dimensional harmonic oscillator is

$$K(x,x';t) = \left(\frac{m\omega}{2\pi i\hbar \sin \omega t} \right)^{1/2} \exp \left(-\frac{m\omega((x^2 + x'^2)\cos \omega t - 2xx')}{2i\hbar \sin \omega t} \right).$$

Time evolution of the wavefunction

apply propagator to starting wavefunction

$$\psi(x,t) = \int U(x,t;x',t')\,\psi(x',t')\,dx'$$

time-dependent wavefcn — propagator — starting wavefcn

$$\boxed{\begin{array}{l} \text{if } \psi(x',t') = \delta(x-x') \\ \text{then } \psi(x,t) = U(x,t;x',t') \\ \text{GAUSSIAN SPREAD} \end{array}}$$

Gaussian spread

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

Probability = wavefcn squared

expectation value of position

Ehrenfest's Theorem

$$\langle x(t)\rangle = \frac{p_0}{m}t = \frac{\langle p\rangle}{m}t \qquad \langle p(t)\rangle = p_0$$

$$\Delta x(t) = \frac{\Delta}{\sqrt{2}}\left(1 + \frac{\hbar^2 t^2}{m^2\Delta^4}\right)^{1/2} \qquad \Delta p(t) = \frac{\hbar}{\sqrt{2}\,\Delta}$$

uncertainty in position

no time dependence

SO AT LONG TIMES

$$\Delta x(t) = \frac{\Delta}{\sqrt{2}}\frac{\hbar t}{m\Delta^2} = A\,t$$

linear in time

$$\Delta x(t) \to \Delta v(0)\,t$$

classical spread

Ehrenfest's Theorem: The expectation values of the quantum variables follow the classical equations of motion

x = v t

Start with a Gaussian envelope in x

$$\psi(x,0) \sim e^{-x^2/2\Delta^2}$$

GAUSSIAN ENVELOPE

MIN WIDTH $\Rightarrow$ $\Delta x = \frac{\Delta}{\sqrt{2}}$

the position distribution depends on time

TIME-DEPENDENT WIDTH

$$\boxed{\Delta x(t) = \frac{\Delta}{\sqrt{2}}\sqrt{1+\frac{\hbar^2 t^2}{m^2\Delta^4}}}$$

AT $t=0$ $\Delta x = \frac{\Delta}{\sqrt{2}}$

WHEN $\frac{\hbar^2 t^2}{m^2\Delta^4} \gg 1$ $\Delta x(t) = \left(\frac{\Delta}{\sqrt{2}}\ \frac{\hbar}{m\Delta^2}\right) t$

$\sim \frac{t}{\Delta}$ SMALLER $\Delta \Rightarrow$ FASTER SPREAD

the momentum distribution is independent of time

$\Delta p(t) = \frac{\hbar}{\sqrt{2}\,\Delta}$ CONSTANT

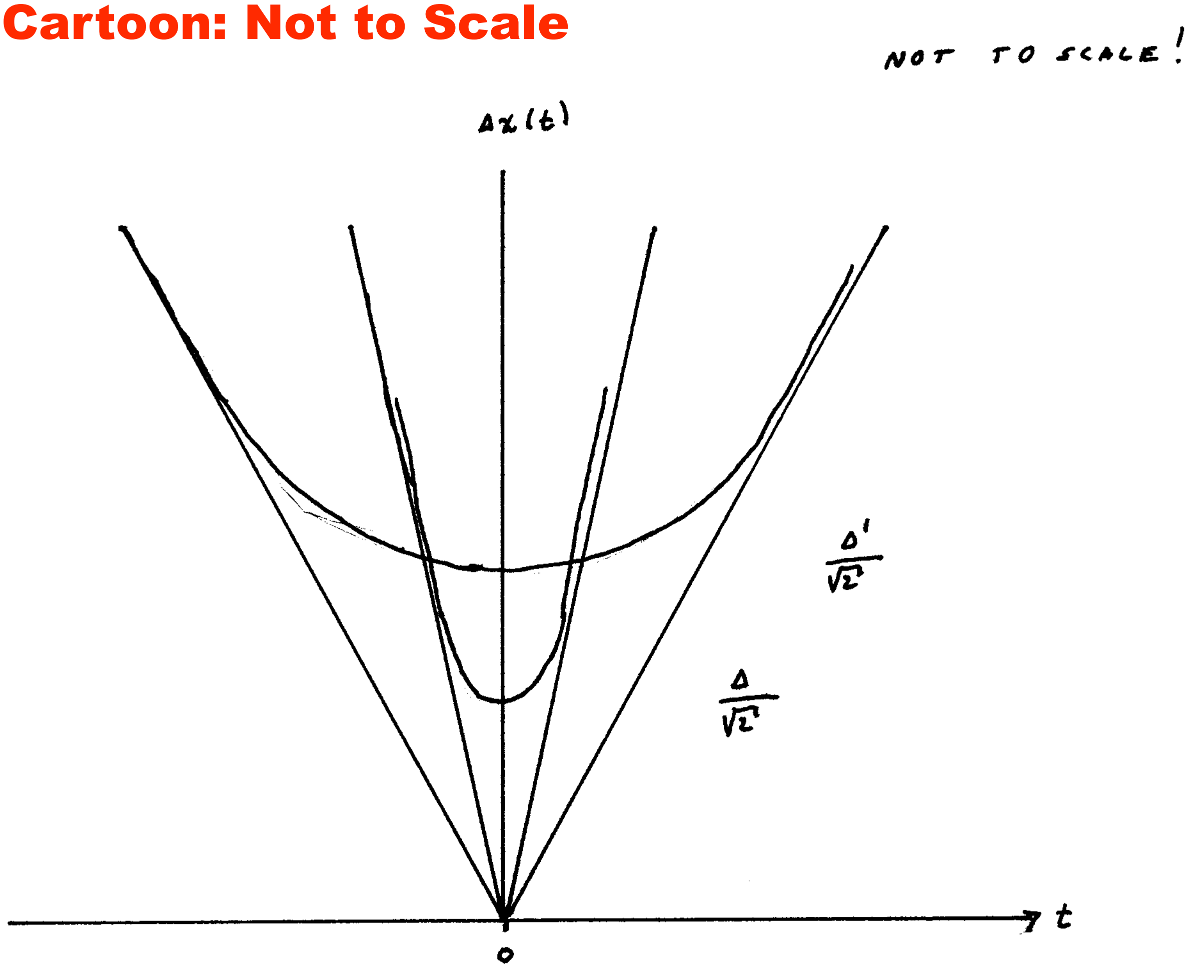
$\Delta v = \frac{\hbar}{\sqrt{2}\, m\Delta}$ SMALLER $\Delta \Rightarrow$ LARGE Δv

CLASSICAL SPREAD

$$\boxed{\Delta x(t) = \Delta v\ t}$$

at long times the quantum spread is the same as the classical spread

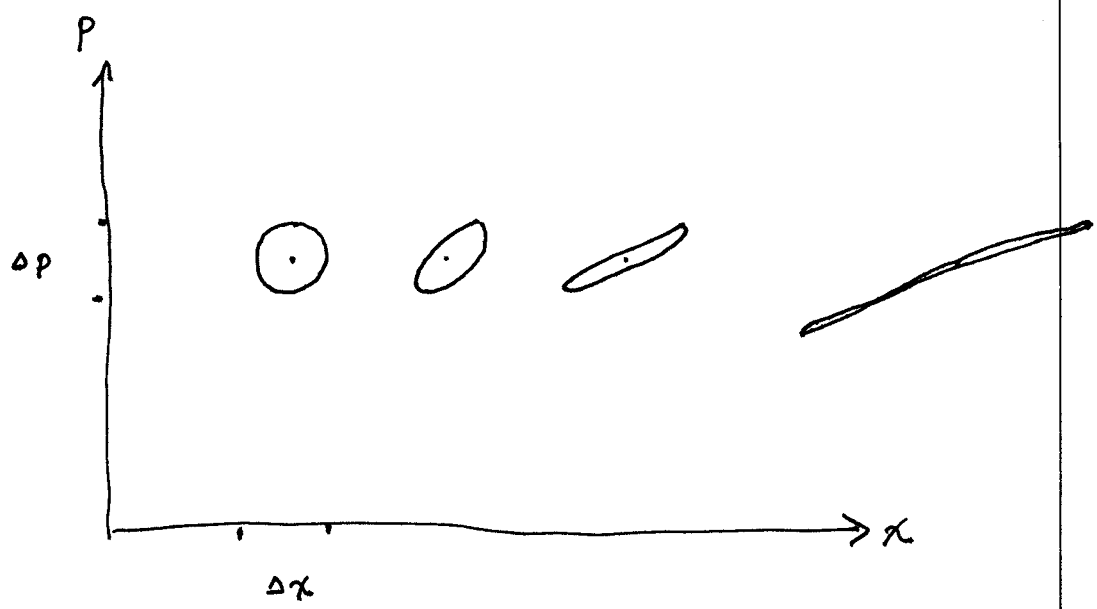
Cartoon: Not to Scale



if the minimum width is small, then the spread is fast

if the minimum width is large, then the spread is slow

CLASSICAL PHASE SPACE



Dispersion

=> Delta x changes

free particle => no forces

=> Delta p stays fixed

FREE PARTICLE

$$\Omega |\omega\rangle = \omega |\omega\rangle$$

OPERATOR ef's ev's

FORM IN ANY BASIS

POSITION SPACE = POSITION BASIS

MOMENTUM SPACE = MOMENTUM BASIS

IN POSITION SPACE

TWO CLASSICAL OBSERVABLES

POSITION	X_{op}	ev's	ef's
MOMENTUM	P_{op}	ev's	ef's

$$X_{op}\, f(x) = x\, f(x)$$

$$P_{op}\, f(x) = -i\hbar \frac{\partial}{\partial x} f(x)$$

DO X AND P COMMUTE?

IS $[x, p] = 0$?

[x, p] is called the canonical commutator fundamental commutator

$xp - px$

$$op = (x)\left(-i\hbar \frac{\partial}{\partial x}\right) - \left(-i\hbar \frac{\partial}{\partial x}\right)(x)$$

DOES $x \frac{\partial}{\partial x} = \frac{\partial}{\partial x} x$

$$x \frac{\partial f}{\partial x} \qquad \frac{\partial}{\partial x}(x f) = \frac{\partial x}{\partial x} f + x \frac{\partial f}{\partial x}$$

NO! THEY DO NOT COMMUTE!

$$x_{op}\, p_{op} - p_{op}\, x_{op} = i\hbar I$$

X AND P ARE COMPLETELY INCOMPATIBLE

$[\ ,\ ] \sim I$ COMP INCOMPATIBLE

$[\ ,\ ] = 0$ COMP COMPATIBLE

IN MOMENTUM SPACE

$$q(p)$$

$$X_{op}\, q(p) = i\hbar \frac{\partial}{\partial p} q(p)$$

$$P_{op}\, q(p) = p\, q(p)$$

DO THEY COMMUTE?

NO

$$\left(p \frac{\partial}{\partial p}\right) q \neq \left(\frac{\partial}{\partial p} p\right) q$$

$$[X_{op}, P_{op}] = i\hbar I$$ COMPLETELY INCOMPATIBLE

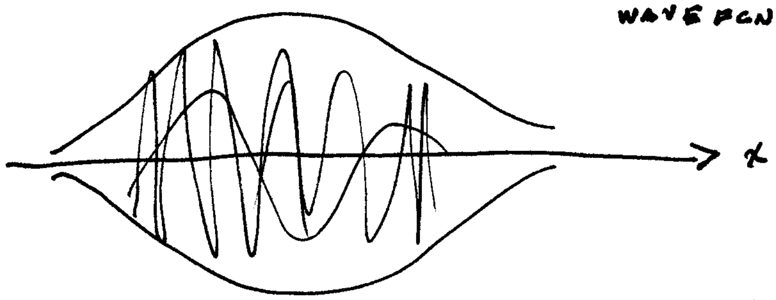
the commutator does not depend on the basis!

it tells us something fundamental about the operators

WHAT ARE THE ef's OF x_{op} FOR THE FREE PARTICLE

before you measure

WAVE FCN

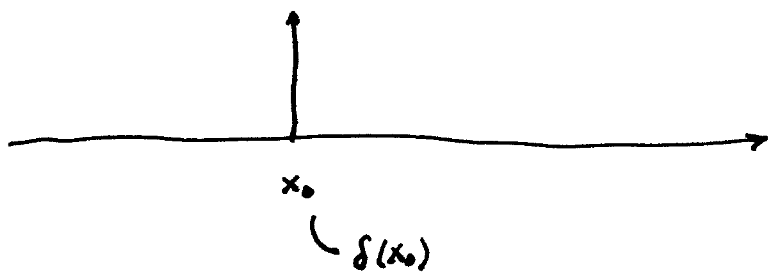


PROB DENSITY

$\int \frown \, dx = 1$

after you measure

AFTER YOU MEASURE



$\int \uparrow dx = 1$

THIS IS CALLED A DIRAC DELTA FCN

∞ HIGH

∞ NARROW

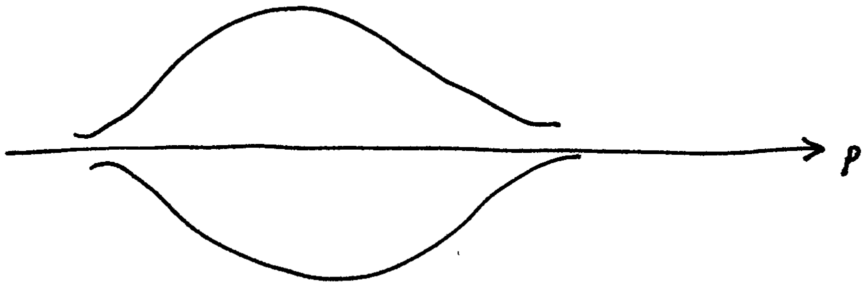
$\int \uparrow \, dx = 1$

In momentum space

WHAT ARE THE ef's OF THE P_{op}

before you measure

WAVEFCN

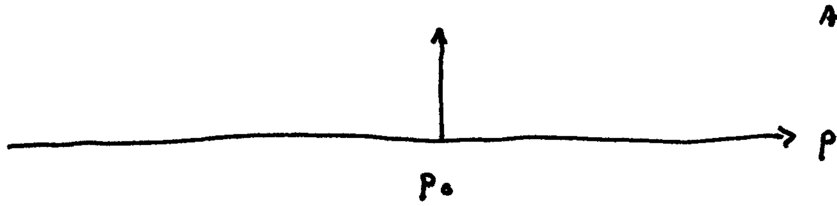


PROB DENSITY

$\int \sim dp = 1$

after you measure

AFTER YOU MEASURE



$\delta(p_0)$

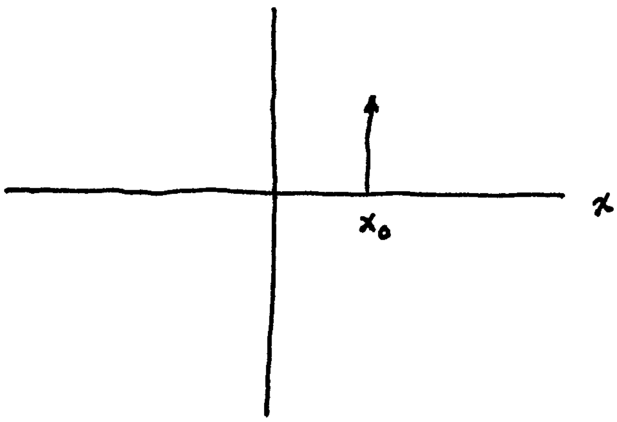
$\int \uparrow dp = 1$

MEASURE X ALWAYS $\delta(x_0)$

MEASURE p ALWAYS $\delta(p_0)$

WHAT DOES $\delta(x_0)$ LOOK LIKE IN p-space?

a delta function in position space



SPATIAL FREQ

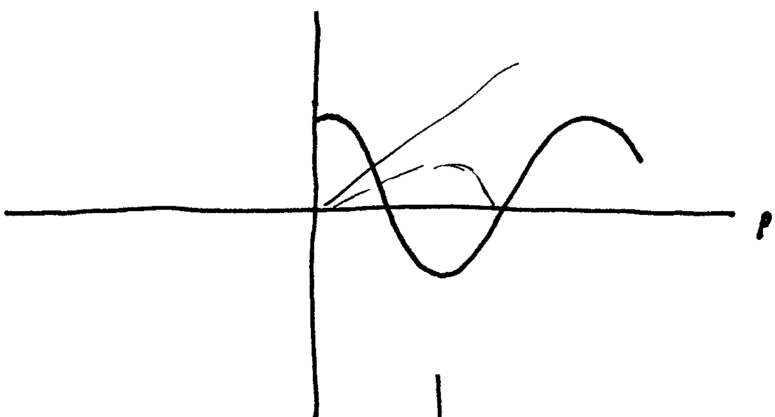
MOMENTUM

$\hbar k = p$

$k = p/\hbar$

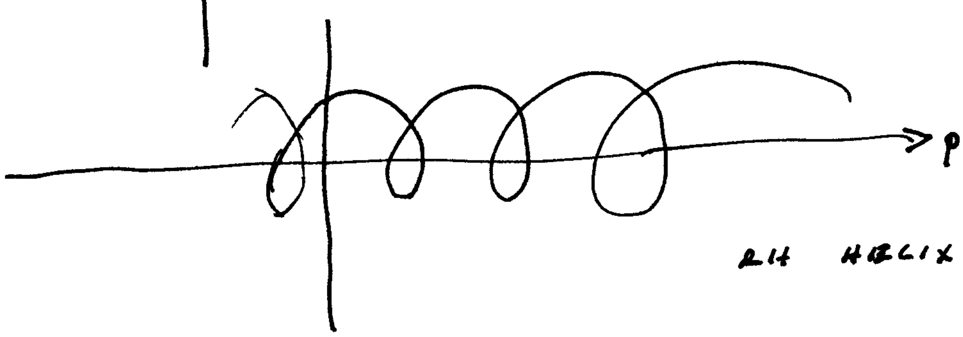
$e^{i p x_0/\hbar}$

$\cos(px/\hbar) + i \sin(px/\hbar)$



real part ~ cos

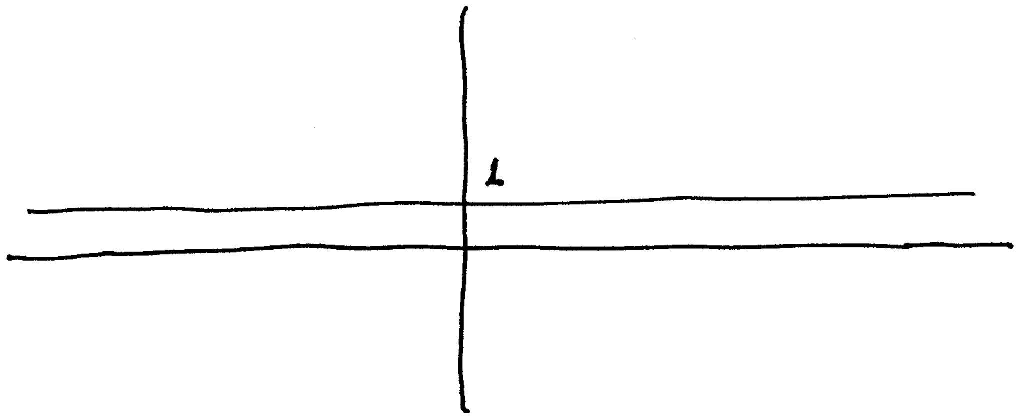
imag part ~ sin



is a helix in momentum space

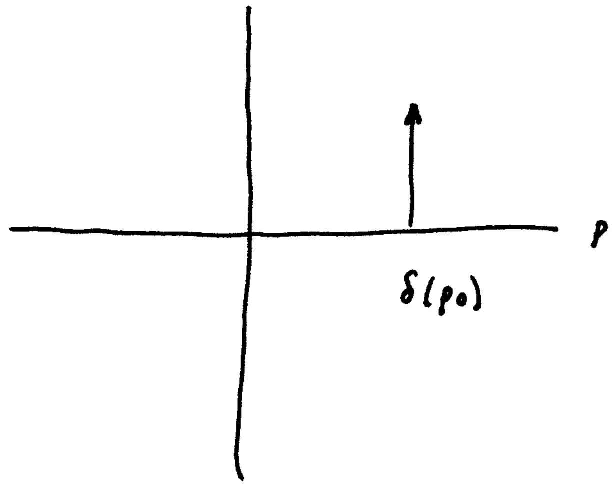
The probability density for a helix

PROB DENSITY $\left| e^{ipx_0/\hbar} \right|^2$



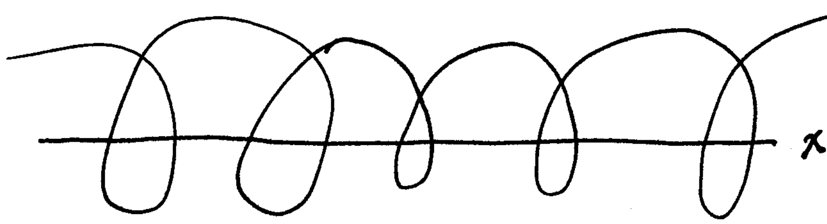
equal probability to find • with any p!

MEASURE p



in momentum space

$$e^{i p_0 x/\hbar}$$



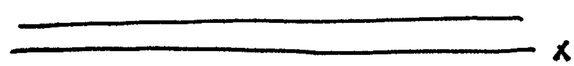
in position space

EQUAL PROBABILITY TO FIND

AT EVERY X

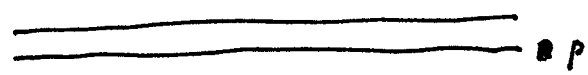
before in x

measure p

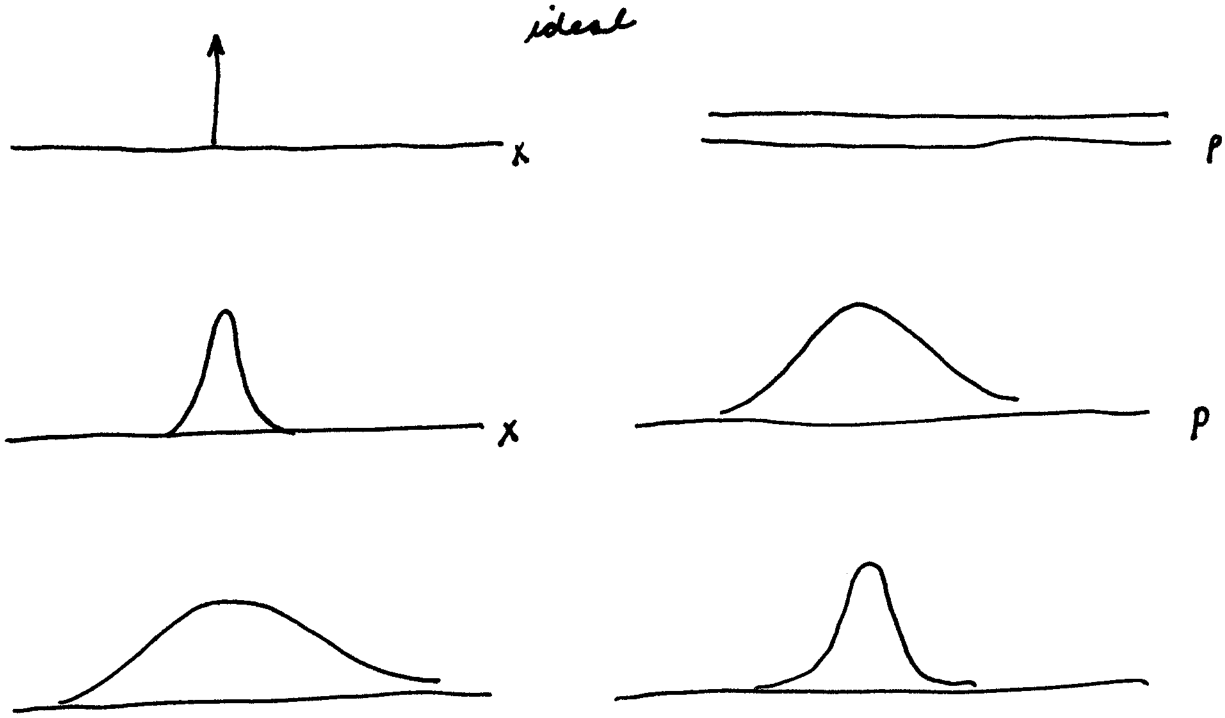


before in p

measure x



CANNOT REALLY DO A PERFECT x OR p MEASUREMENT



$$\Delta x \, \Delta p \geq \hbar/2$$

5

Simple Problems in One Dimension

Now that the postulates have been stated and explained, it is all over but for the applications. We begin with the simplest class of problems—concerning a single particle in one dimension. Although these one-dimensional problems are somewhat artificial, they contain most of the features of three-dimensional quantum mechanics but little of its complexity. One problem we will not discuss in this chapter is that of the harmonic oscillator. This problem is so important that a separate chapter has been devoted to its study.

5.1. The Free Particle

The simplest problem in this family is of course that of the free particle. The Schrödinger equation is

$$i\hbar\,|\dot{\psi}\rangle = H\,|\psi\rangle = \frac{P^2}{2m}\,|\psi\rangle \tag{5.1.1}$$

The normal modes or stationary states are solutions of the form

$$|\psi\rangle = |E\rangle e^{-iEt/\hbar} \tag{5.1.2}$$

Feeding this into Eq. (5.1.1), we get the time-independent Schrödinger equation for $|E\rangle$:

$$H\,|E\rangle = \frac{P^2}{2m}\,|E\rangle = E\,|E\rangle \tag{5.1.3}$$

This problem can be solved without going to any basis. First note that any eigenstate of P is also an eigenstate of P^2. So we feed the trial solution $|p\rangle$ into Eq. (5.1.3) and find

$$\frac{P^2}{2m}\,|p\rangle = E\,|p\rangle$$

or

$$\left(\frac{p^2}{2m} - E\right) |p\rangle = 0 \qquad (= |0\rangle) \tag{5.1.4}$$

Since $|p\rangle$ is not a null vector, we find that the allowed values of p are

$$p = \pm(2mE)^{1/2} \tag{5.1.5}$$

In other words, there are two orthogonal eigenstates for each eigenvalue E:

$$|E, +\rangle = |p = (2mE)^{1/2}\rangle \tag{5.1.6}$$

$$|E, -\rangle = |p = -(2mE)^{1/2}\rangle \tag{5.1.7}$$

Thus, we find that to the eigenvalue E there corresponds a degenerate two-dimensional eigenspace, spanned by the above vectors. Physically this means that a particle of energy E can be moving to the right or to the left with momentum $|p| = (2mE)^{1/2}$. Now, you might say, "This is exactly what happens in classical mechanics. So what's new?" What is new is the fact that the state

$$|E\rangle = \beta\,|p = (2mE)^{1/2}\rangle + \gamma\,|p = -(2mE)^{1/2}\rangle \tag{5.1.8}$$

is also an eigenstate of energy E and represents a *single* particle of energy E that can be caught moving either to the right or to the left with momentum $(2mE)^{1/2}$!

To construct the complete orthonormal eigenbasis of H, we must pick from each degenerate eigenspace any two orthonormal vectors. The obvious choice is given by the kets $|E, +\rangle$ and $|E, -\rangle$ themselves. In terms of the ideas discussed in the past, we are using the eigenvalue of a compatible variable P as an extra label within the space degenerate with respect to energy. Since P is a nondegenerate operator, the label p by itself is adequate. In other words, there is no need to call the state $|p, E = p^2/2m\rangle$, since the value of $E = E(p)$ follows, given p. We shall therefore drop this redundant label.

The propagator is then

$$\begin{aligned} U(t) &= \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-iE(p)t/\hbar}\, dp \\ &= \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-ip^2t/2m\hbar}\, dp \end{aligned} \tag{5.1.9}$$

Exercise 5.1.1. Show that Eq. (5.1.9) may be rewritten as an integral over E and a sum over the $\pm$ index as

$$U(t)=\sum_{\alpha=\pm}\int_0^\infty\left[\frac{m}{(2mE)^{1/2}}\right]|E,\alpha\rangle\langle E,\alpha|\,e^{-iEt/\hbar}\,dE$$

*Exercise 5.1.2.** By solving the eigenvalue equation (5.1.3) in the X basis, regain Eq. (5.1.8), i.e., show that the general solution of energy E is

$$\psi_E(x)=\beta\,\frac{\exp[i(2mE)^{1/2}x/\hbar]}{(2\pi\hbar)^{1/2}}+\gamma\,\frac{\exp[-i(2mE)^{1/2}x/\hbar]}{(2\pi\hbar)^{1/2}}$$

[The factor $(2\pi\hbar)^{-1/2}$ is arbitrary and may be absorbed into β and γ.] Though $\psi_E(x)$ will satisfy the equation even if $E<0$, are these functions in the Hilbert space?

The propagator $U(t)$ can be evaluated explicitly in the X basis. We start with the matrix element

$$\begin{aligned}U(x,t;x')\equiv\langle x|U(t)|x'\rangle&=\int_{-\infty}^{\infty}\langle x|p\rangle\langle p|x'\rangle e^{-ip^2t/2m\hbar}\,dp\\&=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{ip(x-x')/\hbar}\cdot e^{-ip^2t/2m\hbar}\,dp\\&=\left(\frac{m}{2\pi\hbar it}\right)^{1/2}e^{im(x-x')^2/2\hbar t}\end{aligned}\tag{5.1.10}$$

using the result from Appendix A.2 on Gaussian integrals. In terms of this propagator, any initial-value problem can be solved, since

$$\psi(x,t)=\int U(x,t;x')\psi(x',0)\,dx'\tag{5.1.11}$$

Had we chosen the initial time to be t' rather than zero, we would have gotten

$$\psi(x,t)=\int U(x,t;x',t')\psi(x',t')\,dx'\tag{5.1.12}$$

where $U(x,t;x',t')=\langle x|U(t-t')|x'\rangle$, since U depends only on the time interval $t-t'$ and not the absolute values of t and t'. [Had there been a time-dependent potential such as $V(t)=V_0e^{-\alpha t^2}$ in H, we could have told what absolute time it was by looking at $V(t)$. In the absence of anything defining an absolute time in the problem, only time differences have physical significance.] Whenever we set $t'=0$, we will resort to our old convention and write $U(x,t;x',0)$ as simply $U(x,t;x')$.

A nice physical interpretation may be given to $U(x, t; x', t')$ by considering a special case of Eq. (5.1.12). Suppose we started off with a particle localized at $x' = x_0'$, that is, with $\psi(x', t') = \delta(x' - x_0')$. Then

$$\psi(x, t) = U(x, t; x_0', t') \tag{5.1.13}$$

In other words, the propagator (in the X basis) is the amplitude that a particle starting out at the space–time point (x_0', t') ends with at the space–time point (x, t). [It can obviously be given such an interpretation in any basis: $\langle \omega \mid U(t, t') \mid \omega' \rangle$ is the amplitude that a particle in the state $\mid \omega' \rangle$ at t' ends up with in the state $\mid \omega \rangle$ at t.] Equation (5.1.12) then tells us that the total amplitude for the particle's arrival at (x, t) is the sum of the contributions from all points x' with a weight proportional to the initial amplitude $\psi(x', t')$ that the particle was at x' at time t'. One also refers to $U(x, t; x_0't')$ as the "fate" of the delta function $\psi(x', t') = \delta(x' - x_0')$.

Time Evolution of the Gaussian Packet

There is an unwritten law which says that the derivation of the free-particle propagator be followed by its application to the Gaussian packet. Let us follow this tradition.

Consider as the initial wave function the wave packet

$$\psi(x', 0) = e^{ip_0x'/\hbar} \frac{e^{-x'^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}} \tag{5.1.14}$$

This packet has mean position $\langle X \rangle = 0$, with an uncertainty $\Delta X = \Delta/2^{1/2}$, and mean momentum p_0 with uncertainty $\hbar/2^{1/2}\Delta$. By combining Eqs. (5.1.10) and (5.1.12) we get

$$\begin{aligned}\psi(x, t) = {} & \left[\pi^{1/2}\left(\Delta + \frac{i\hbar t}{m\Delta}\right)\right]^{-1/2} \cdot \exp\left[\frac{-(x - p_0t/m)^2}{2\Delta^2(1 + i\hbar t/m\Delta^2)}\right] \\ & \times \exp\left[\frac{ip_0}{\hbar}\left(x - \frac{p_0t}{2m}\right)\right]\end{aligned} \tag{5.1.15}$$

The corresponding probability density is

$$P(x, t) = \frac{1}{\pi^{1/2}(\Delta^2 + \hbar^2t^2/m^2\Delta^2)^{1/2}} \cdot \exp\left\{\frac{-[x - (p_0/m)t]^2}{\Delta^2 + \hbar^2t^2/m^2\Delta^2}\right\} \tag{5.1.16}$$

The main features of this result are as follows:

(1) The mean position of the particles is

$$\langle X \rangle = \frac{p_0 t}{m} = \frac{\langle P \rangle t}{m}$$

In other words, the classical relation $x = (p/m)t$ now holds between average quantities. This is just one of the consequences of the *Ehrenfest theorem* which states that the classical equations obeyed by dynamical variables will have counterparts in quantum mechanics as relations among expectation values. The theorem will be proved in the next chapter.

(2) The width of the packet grows as follows:

$$\Delta X(t) = \frac{\Delta(t)}{2^{1/2}} = \frac{\Delta}{2^{1/2}} \left(1 + \frac{\hbar^2 t^2}{m^2 \Delta^4}\right)^{1/2} \tag{5.1.17}$$

The increasing uncertainty in position is a reflection of the fact that any uncertainty in the initial velocity (that is to say, the momentum) will be reflected with passing time as a growing uncertainty in position. In the present case, since $\Delta V(0) = \Delta P(0)/m = \hbar/2^{1/2}m\Delta$, the uncertainty in X grows approximately as $\Delta X \simeq \hbar t/2^{1/2}m\Delta$ which agrees with Eq. (5.1.17) for large times. Although we are able to understand the spreading of the wave packet in classical terms, the fact that the initial spread $\Delta V(0)$ is *unavoidable* (given that we wish to specify the position to an accuracy Δ) is a purely quantum mechanical feature.

If the particle in question were macroscopic, say of mass 1 g, and we wished to fix its initial position to within a proton width, which is approximately 10^{-13} cm, the uncertainty in velocity would be

$$\Delta V(0) \simeq \frac{\hbar}{2^{1/2} m\Delta} \simeq 10^{-14} \text{ cm/sec}$$

It would be over 300,000 years before the uncertainty $\Delta(t)$ grew to one millimeter! We may therefore treat a macroscopic particle classically for any reasonable length of time. This and similar questions will be taken up in greater detail in the next chapter.

Exercise 5.1.3. (*Another Way to Do the Gaussian Problem*). We have seen that there exists another formula for $U(t)$, namely, $U(t) = e^{-iHt/\hbar}$. For a free particle this becomes

$$U(t) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2 t}{2m}\frac{d^2}{dx^2}\right)\right] = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{i\hbar t}{2m}\right)^n \frac{d^{2n}}{dx^{2n}} \tag{5.1.18}$$

LECTURE 18 JULY 23, 2007

SOLVE SHO DIFF EQ

$$\boxed{H \mid \varphi_n \rangle = E_n \mid \varphi_n \rangle}$$

TISE in Dirac notation for the SHO

to get x-space, dot with $\langle x \mid$ bra

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2\right]\varphi_n(x) = E_n\,\varphi_n(x)$$

Find ev's E_n **eigenvalues**

Find ef's $\varphi_n(x)$ **eigenfunctions**

TISE in position space

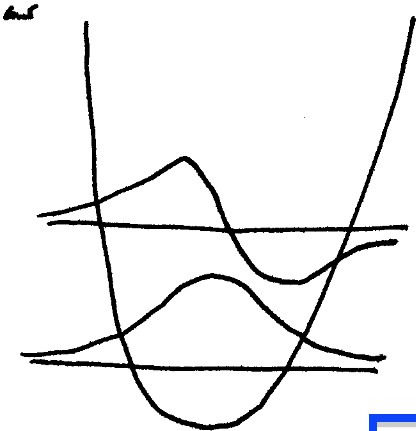
TELL 'EM WHAT YOU'RE GONNA TELL 'EM

ZERO CROSSINGS

2

1

0



second excited state has 2 zeros

first excited state has 1 zero

ground state has no zeros

FIND ASYPTOTIC FORM OUTSIDE

≈ GAUSSIAN

SOLUTION = GAUSSIAN × POLYNOMIALS

HERMITE POLYNOMIALS

Lecture 11

SOLVE TISE IN POSITION SPACE

$H|n\rangle = E_n|n\rangle$ **in Dirac notation**

OPERATOR IN x-SPACE

EIGENENERGIES

WAVE FUNCTIONS $\varphi_n(x)$ IN x-SPACE

FOUND $E_n = (n + 1/2)\hbar\omega \qquad n = 0, 1, 2, 3, \dots$

in position space $\varphi_n(y) = H_n(y)\, e^{-y^2/2}$

STATIONARY STATES

AKA

ENERGY EIGENFUNCTIONS

HERMITE POLYNOMIALS

GAUSSIAN

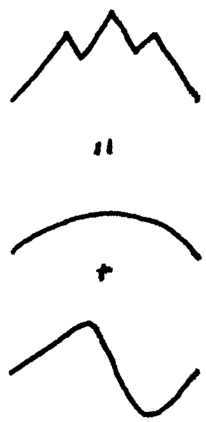
Eigenfunctions of H are a complete set of functions

http://www.st-andrews.ac.uk/~qmanim/animations_2/

THE EIGENFUNCTIONS OF THE HAMILTONIAN ARE A COMPLETE ORTHONORMAL SET OF BASIS FUNCTIONS FOR THE SPACE

SQUARE WELL

INTERVAL:



ANY FUNCTION

FOURIER SERIES

Square Well

space = interval

weight fcns = constant

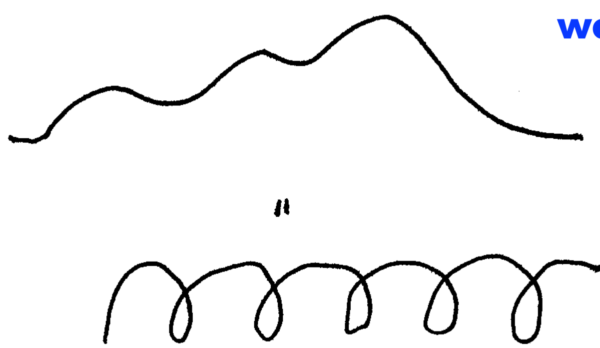
$$\psi(x) = \sum_{m} a_m e^{ik_m x}$$

Free Particle

space = line

weight fcns = constant

LINE: FREE PARTICLE



ANY FUNCTION

FOURIER INTEGRAL

$$\psi(x) = \int \hat{\psi}(p) \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} dp$$

$$\psi(x) = (2\pi)^{-1/2} \int a(k) e^{ikx} dk$$

$$\int e^{-ikx} e^{ik'x} dx = \delta(k'-k)$$

HARMONIC OSCILLATOR

Simple Harmonic Oscillator

space = line

weight fcns = Gaussians

LINE: HERMITE FUNCTIONS

$$\int H_n(x)\, H_m(x)\, e^{-x^2}\, dx = \delta_{nm}$$

Hermite Polynomials

$$f(x) = \sum_n a_n H_n(x)$$

HYDROGEN ATOM

Hydrogen Atom

space = half line

weight fcns = exponentials

HALF-LINE

LAGUERRE POLYNOMIALS

$$\int_0^\infty L_n(r)\, L_m(r)\, e^{-r}\, dr = \delta_{nm}$$

Laguerre Polynomials

IN DIRAC NOTATION, ALL OF THE ABOVE ARE

$$|\psi\rangle = I\, |\psi\rangle$$

$$= \sum |n\rangle \underbrace{\langle n|\psi\rangle}_{a_n}$$

$$|\psi\rangle = \sum a_n |n\rangle$$

$$\langle n|m\rangle = \delta_{nm}$$

TODAY: SHO-2 POWER SERIES, ORTHOGONAL POLYNOMIALS, DIFFERENTIAL EQUATIONS, AND ALL THAT....

WE WANT TO SOLVE TDSE

$$H|\psi\rangle = i\hbar \frac{d}{dt}|\psi\rangle$$

To solve TDSE

SO WE FIRST SOLVE TISE

$$H|E_m\rangle = E_m|E_m\rangle$$

First solve TISE

Then use the time-dependent phase factors of

THEN USE **the energy eigenkets/eigenvectors/eigenfunctions**

$$|\psi(t)\rangle = \underbrace{\boxed{\sum_m |E_m\rangle\langle E_m| \, e^{-iE_m t/\hbar}}}_{\text{Propagator } U(t)} |\psi(0)\rangle$$

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

SO, TO SOLVE TISE...

LECTURE 11: SHO II

POWER SERIES, DIFF EQ'S, AND ALL THAT

TISE

in Dirac notation

in the Hilbert space

$$H \,|\, \varphi_n \rangle = E_n \,|\, \varphi_n \rangle$$

using position basis:

The TISE is a differential equation in position space

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} k x^2 \right] \varphi_n(x) = E_n \, \varphi_n(x)$$

OUR JOB: FIND φ_n's **eigenfunctions**

FIND E_n's **eigenvalues**

REWRITE TISE

$$\frac{d^2 \psi}{dx^2} + (\lambda - \alpha^2 x^2)\, \psi = 0$$

$$\lambda = \frac{2mE}{\hbar^2}$$

$$\alpha = \frac{mk}{\hbar^2}$$

make a bunch of variable changes to make it look like some old dead guy's differential equation, then we will pretend to solve it

FIRST STEP: FIND ASYMPTOTIC SOLUTION

FOR LARGE x, $\quad \alpha^2 x^2 \gg \lambda$

$$\frac{d^2\psi}{dx^2} - \alpha^2 x^2 \psi = 0$$

Trial solutions from the freshman physics professors

$$\psi = A e^{-\frac{1}{2}\alpha x^2} + B e^{+\frac{1}{2}\alpha x^2}$$

$$\frac{d\psi}{dx} = -\alpha x \, A e^{-\frac{1}{2}\alpha x^2} + \alpha x \, B e^{+\frac{1}{2}\alpha x^2}$$

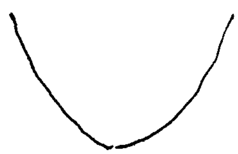
$$\frac{d^2\psi}{dx^2} = \alpha^2 x^2 A e^{-\frac{1}{2}\alpha x^2} + \alpha^2 x^2 B e^{+\frac{1}{2}\alpha x^2}$$

$$\cancel{- \alpha A e^{-\frac{1}{2}\alpha x^2}} + \cancel{\alpha B e^{+\frac{1}{2}\alpha x^2}}$$

Yes, they are indeed solutions to the asymptotic equation!

$\alpha^2 x^2 \gg \alpha$

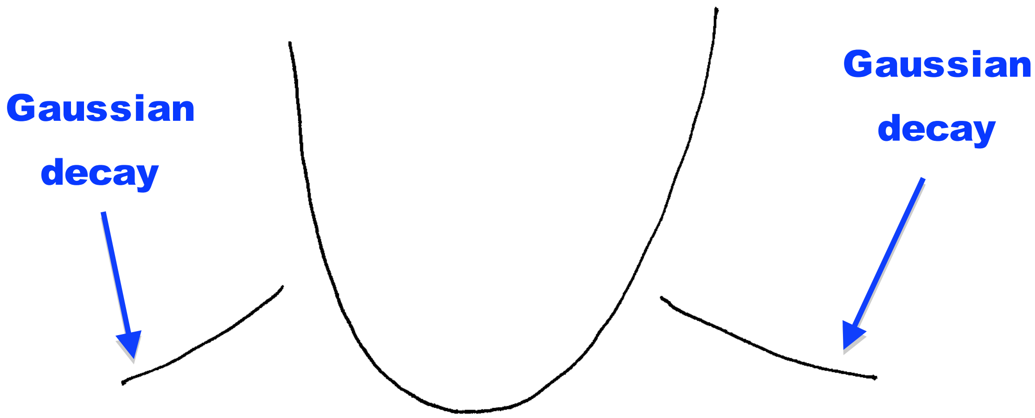
$$\boxed{\begin{aligned} \psi(x) &= A \, e^{-\frac{1}{2}\alpha x^2} \\ \psi(x) &= B \, e^{+\frac{1}{2}\alpha x^2} \end{aligned}}$$



not physical at infinity

not square integ

SO, AT LARGE x, WE HAVE GAUSSIAN DECAY



LOOK FOR SOLUTIONS OF THE FORM

$$\boxed{\psi(x) = e^{-\frac{1}{2}\alpha x^2} f(x)}$$

Trial solution to remove the asymptotic part

$$\frac{d^2\psi}{dx^2} + (\lambda - \alpha^2 x^2)\,\psi = 0$$

Put in the trial solution and do all of the spatial derivatives

$$\frac{d\psi}{dx} = \frac{d}{dx}\left[e^{-\frac{1}{2}\alpha x^2} f(x) \right]$$

$$= -\alpha x\, e^{-\frac{1}{2}\alpha x^2} f(x) + e^{-\frac{1}{2}\alpha x^2} \frac{df}{dx}$$

$$\frac{d^2\psi}{dx^2} = -\alpha e^{-\frac{1}{2}\alpha x^2} f(x) + \alpha^2 x^2 e^{-1/2\,\alpha x^2} f(x)$$

$$- \alpha x e^{-1/2\,\alpha x^2} \frac{df}{dx} - \alpha x e^{-1/2\,\alpha x^2} \frac{df}{dx}$$

$$+ e^{-\frac{1}{2}\alpha x^2} \frac{d^2 f}{dx^2}$$

$$\frac{d^2\psi}{dx^2} \Rightarrow \left[\frac{d^2 f}{dx^2} - 2\alpha x \frac{df}{dx} + (\cancel{\alpha^2 x^2} - \alpha) f \right] e^{-1/2\,\alpha x^2}$$

$$+ (\lambda - \alpha^2 x^2)\psi = 0$$

$$+ (\lambda - \cancel{\alpha^2 x^2}) f e^{-1/2\,\alpha x^2} = 0$$

Okay, the equation inside the [ ] must be zero

$$0 = \left[\frac{d^2 f}{dx^2} - 2\alpha x \frac{df}{dx} + (\lambda - a) f \right] \cancel{e^{-1/2\,\alpha x^2}}$$

It doesn't look exactly like the old dead guy's differential equation, so make some more variable changes

$$\xi = \sqrt{\alpha}\, x$$

$$f(x) \rightarrow H(\xi)$$

$$\frac{d}{dx} f(x) = \frac{d}{dx} H(\xi) = \frac{d}{d\xi} H(\xi) \frac{d\xi}{dx}$$

$$= \frac{dH(\xi)}{d\xi} \sqrt{\alpha}$$

$$\frac{d^2 f}{dx^2} = \alpha \frac{d^2 H}{d\xi^2}$$

$$\frac{d^2 f}{dx^2} - 2\alpha x \frac{df}{dx} + (\lambda - \alpha) f = 0$$

$$\frac{1}{\alpha}\left[\alpha \frac{d^2 H}{d\xi^2} - 2\alpha x \frac{dH}{d\xi}\sqrt{\alpha} + (\lambda - \alpha) H\right] = 0$$

$$\xi = \sqrt{\alpha}\, x$$

Success!!! Now it looks exactly like the old dead guy's equation!!!

$$\boxed{\frac{d^2 H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + \left(\frac{\lambda}{\alpha} - 1\right) H = 0}$$

HERMITE'S EQN

Now we pretend to solve the old dead guy's equation

SOLVE USING POWER SERIES ...

$$H(\xi) = a_0 + a_1 \xi + a_2 \xi^2 + a_3 \xi^3 + \dots$$

$$\frac{dH}{d\xi} = 0 + a_1 + 2 a_2 \xi + 3 a_3 \xi^2 + \dots$$

$$\frac{d^2H}{d\xi^2} = 0 + 0 + 1\cdot 2\, a_2 + 2\cdot 3\, a_3 \xi$$

KNOW

$$\frac{d^2H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + \left(\frac{\lambda}{\alpha} - 1\right) H = 0 \qquad \text{FOR ALL } \xi \,!$$

$\Rightarrow$ each coefficient of ξ must vanish

ξ^0 $$1\cdot 2\, a_2 + \left(\frac{\lambda}{\alpha} - 1\right) a_0 = 0$$

ξ^1 $$2\cdot 3\, a_3 + \left(\frac{\lambda}{\alpha} - 1 - 2\right) a_1 = 0$$

ξ^2 $$3\cdot 4\, a_4 + \left(\frac{\lambda}{\alpha} - 1 - 2\cdot 2\right) a_2 = 0$$

ξ^3 $$4\cdot 5\, a_5 + \left(\frac{\lambda}{\alpha} - 1 - 2\cdot 3\right) a_3 = 0$$

$\Rightarrow$ COEFF OF ξ^m

$$(m+1)(m+2)\, a_{m+2} + \left(\frac{\lambda}{\alpha} - 1 - 2m\right) a_m = 0$$

$$\boxed{a_{m+2} = \frac{-\left(\frac{\lambda}{\alpha} - 2m - 1\right)}{(m+2)(m+1)}\, a_m}$$

RECURSION RELATION

Recursion Relation

$\Delta m = 2$ $\quad a_0 \Rightarrow$ all even COEFF'S

$a_1 \Rightarrow$ all ODD COEFF'S

FOR EACH m:

WHEN $\left(+\frac{\lambda}{\alpha} - 2m - 1\right) = 0$

all higher terms vanish!

SPECIAL VALUES OF λ ⇒ FINITE POLYNOMIALS

$$\lambda = \frac{2mE}{\hbar}$$

⇒ EIGENENERGIES !

TWO CLASSES OF SOLUTIONS

in 1d, even and odd solutions

in 3d, even and odd turn into parity

spatial inversion

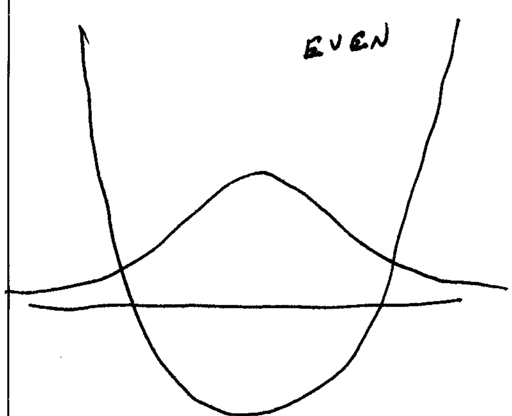
EVEN

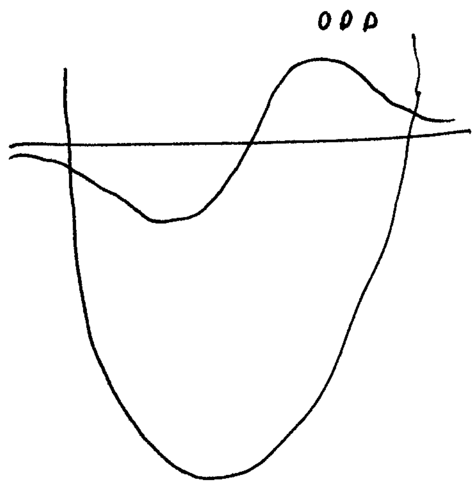
$$H(\xi) = a_0 + a_2 \xi^2 + a_4 \xi^4 + \dots$$

ODD

$$H(\xi) = a_1 \xi + a_3 \xi^3 + a_5 \xi^5 + \dots$$

ODD AND EVEN COME FROM SYMMETRY OF THE PROBLEM





N. B., FOR AN ARBITRARY ENERGY, NO STATIONARY STATE! SERIES ~~DO~~ DOES NOT TERMINATE!

$$a_{m+2} = \frac{-\left[\frac{\lambda}{\alpha} - 2m - 1\right]}{(m+2)(m+1)} a_m$$

CAN CHOOSE λ TO TERMINATE EVEN OR ODD SERIES, BUT NOT BOTH.

LARGE m

$$a_{m+2} = \frac{-\left[\cancel{\frac{\lambda}{\alpha}} - 2m - \cancel{1}\right]}{(m+\cancel{2})(m+\cancel{1})} a_m$$

$$a_{m+2} = +\left(\frac{2}{m}\right) a_m$$

COMPARE WITH POWER SERIES FOR A GAUSSIAN

$$e^{\xi^2} = \sum_{n=0}^{\infty} \frac{(\xi^2)^n}{n!} = 1 + \xi^2 + \frac{1}{2!}\xi^4 + \frac{1}{3!}\xi^6$$

$$+ \frac{\xi^m}{\left(\frac{m}{2}\right)!} + \frac{\xi^{m+2}}{\left(\frac{m+2}{2}\right)!}$$

$$\frac{b_{m+2}}{b_m} = \left(\frac{2}{m}\right) \Rightarrow \text{SAME!}$$

CALCULATE THE EIGENENERGIES

$$\left[\frac{\lambda}{\alpha} - 2m - 1 \right] = 0$$

$$\frac{\lambda}{\alpha} = 2m + 1$$

$$\lambda = (2m+1)\,\alpha$$

$$\frac{2mE}{\hbar^2} = (2m+1)\sqrt{\frac{mK}{\hbar^2}}$$

$$E = (2m+1)\,\frac{\hbar^2}{2m}\sqrt{\frac{mK}{\hbar^2}}$$

$$= (m + 1/2)\,\hbar\sqrt{\frac{K}{m}}$$

$$= (m + 1/2)\,\hbar\,\omega$$

Hermite polynomials

$$
\begin{aligned}
H_0(\xi) &= 1 \\
H_1(\xi) &= 2\xi \\
H_2(\xi) &= 4\xi^2 - 2 \\
H_3(\xi) &= 8\xi^3 - 12\xi \\
H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12 \\
H_5(\xi) &= 32\xi^5 - 160\xi^3 + 120\xi \qquad (11\text{–}23) \\
H_6(\xi) &= 64\xi^6 - 480\xi^4 + 720\xi^2 - 120 \\
H_7(\xi) &= 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi \\
H_8(\xi) &= 256\xi^8 - 3584\xi^6 + 13440\xi^4 - 13440\xi^2 + 1680 \\
H_9(\xi) &= 512\xi^9 - 9216\xi^7 + 48384\xi^5 - 80640\xi^3 + 30240\xi \\
H_{10}(\xi) &= 1024\xi^{10} - 23040\xi^8 + 161280\xi^6 - 403200\xi^4 + 302400\xi^2 \\
&\quad - 30240.
\end{aligned}
$$

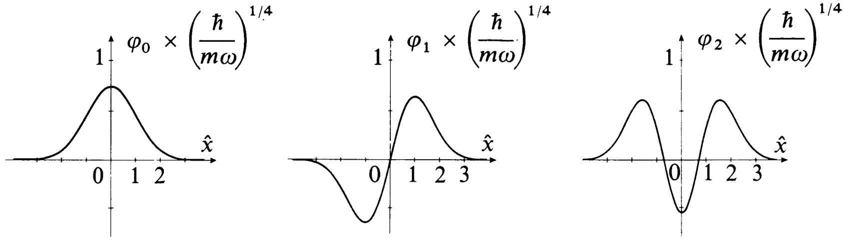


FIGURE 4

Wave functions associated with the first three levels of a harmonic oscillator.

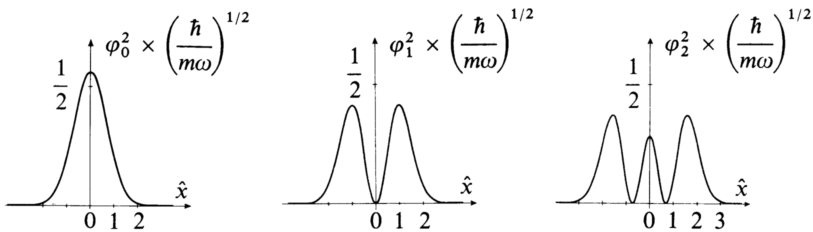


FIGURE 5

Probability densities associated with the first three levels of a harmonic oscillator.

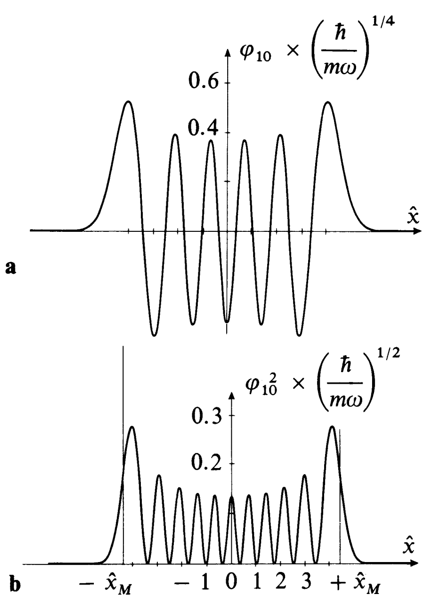


FIGURE 6

Shape of the wave function (fig. a) and of the probability density (fig. b) for the $n = 10$ level of a harmonic oscillator.

The Harmonic Oscillator

http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc.html
http://www.falstad.com/qm1d/
http://www-personal.umich.edu/~lorenzon/java_applets/spaceholder/applets/SHO-QM-example.html?D1=5
http://www.quantum-physics.polytechnique.fr/en/

Hermite Polynomials

http://mathworld.wolfram.com/HermitePolynomial.html
http://www.efunda.com/math/Hermite/index.cfm
http://www.sci.wsu.edu/idea/quantum/hermite.htm
http://functions.wolfram.com/Polynomials/

Coherent States

http://cat.sckans.edu/physics/Quantum%20Wave%20Ppacket.htm http://demonstrations.wolfram.com/FundamentalCommutationRelationsInQuantumMechanics/

http://demonstrations.wolfram.com/SchroedingersCatOnCatnip/

http://www.fen.bilkent.edu.tr/~yalabik/applets/collapse.html