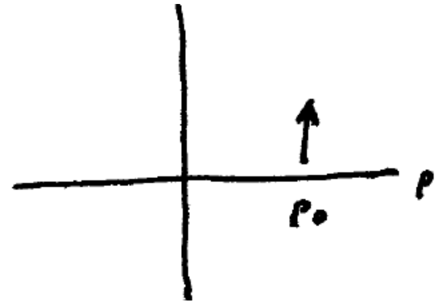
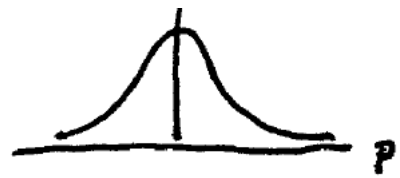
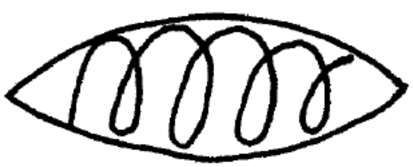
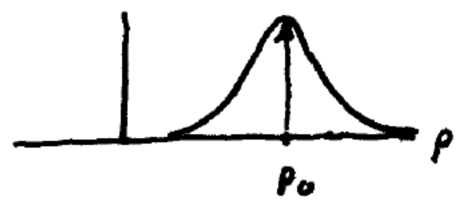
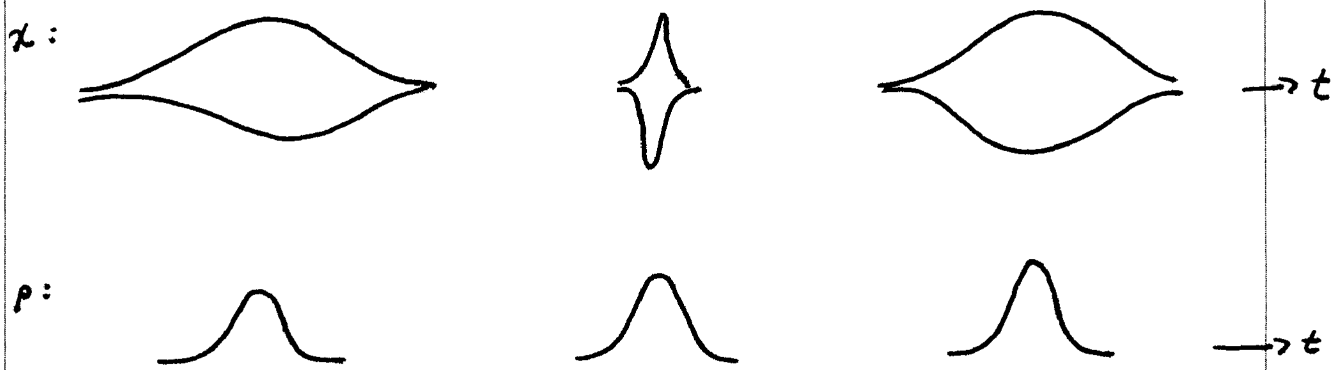
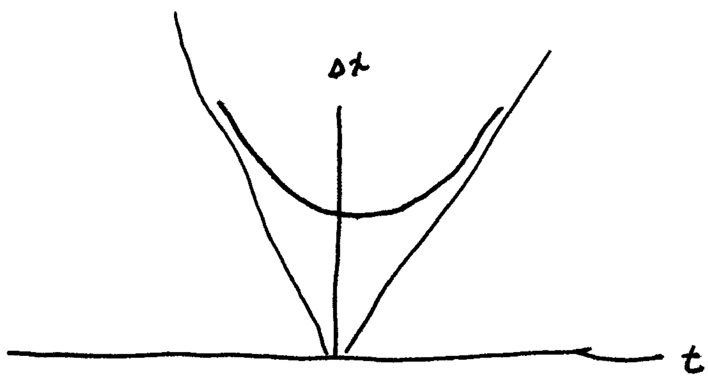
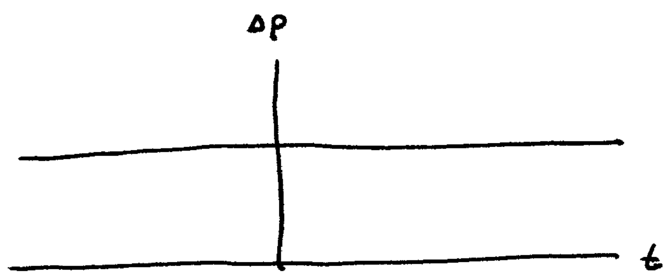
position space		momentum space
A plane wave	<=>	**A delta function at $p=p_o$**
	<=>	
times	<=>	**convolved with**
A Gaussian	<=>	**A Gaussian at p=0**
	<=>	
is equal to	<=>	**is equal to**
A wavepacket	<=>	**A Gaussian at $p=p_o$**
	<=>	


x :
→ t
p :
→ t


Δx
t


Δp
t

(1) FINISH FREE WAVE PACKET

QUANTITATIVE

(2) START HARMONIC OSCILLATOR

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

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 UNCERTAINY AT $t=0$

INCLUDE THE TIME-DEPENDENT PHASE FACTORS

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

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

$$e^{-im(x-x')/2\hbar(t-t')}$$

~~$\psi(x,t) = \int U(x,t)\,\psi($~~

$$U(t) = \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-iE(p)t/\hbar}$$

$$= \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-i(p^2/2m)t/\hbar}$$

STILL IN THE HILBERT SPACE

IN X-SPACE

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

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

$$= \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x')/2\hbar t}$$

$$= U(x,t;x',0)$$

$$= U(x,t;x',t') \qquad t \to t-t'$$

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

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

$$\nabla^2 \psi = \gamma \frac{d\psi}{d(it)}$$

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 time-evolution operator for the system taking states at time t to states at time t'.

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 is

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

.

$$U(t) = \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-iE(p)t/\hbar}$$

$$= \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-i(p^2/2m)t/\hbar}$$

STILL IN THE HILBERT SPACE

IN X-SPACE

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

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

$$= \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x')/2\hbar t}$$

$$= U(x,t;x',0)$$

$$= U(x,t;x',t') \qquad t \to t-t'$$

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

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

$$\nabla^2 \psi = \gamma \frac{d\psi}{d(it)}$$

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

if $\psi(x',t') = \delta(x-x')$

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

GAUSSIAN SPREAD

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

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

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

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

$\Delta x(t) \rightarrow \Delta v(0)\,t$ classical spread

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

GAUSSIAN
ENVELOPE

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

TIME-DEPENDENT WIDTH

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

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

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

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

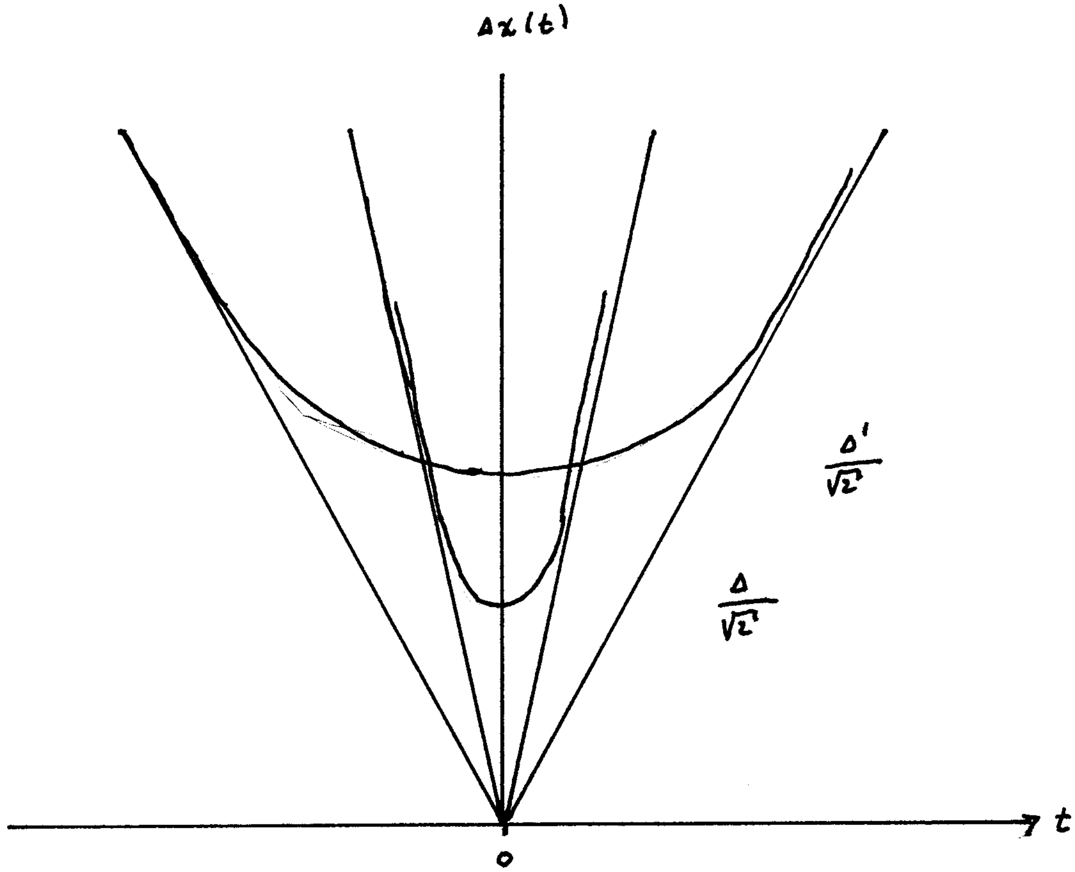
$\Delta p(t) = \frac{\hbar}{\sqrt{2}\,\Delta}$ CONSTANT

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

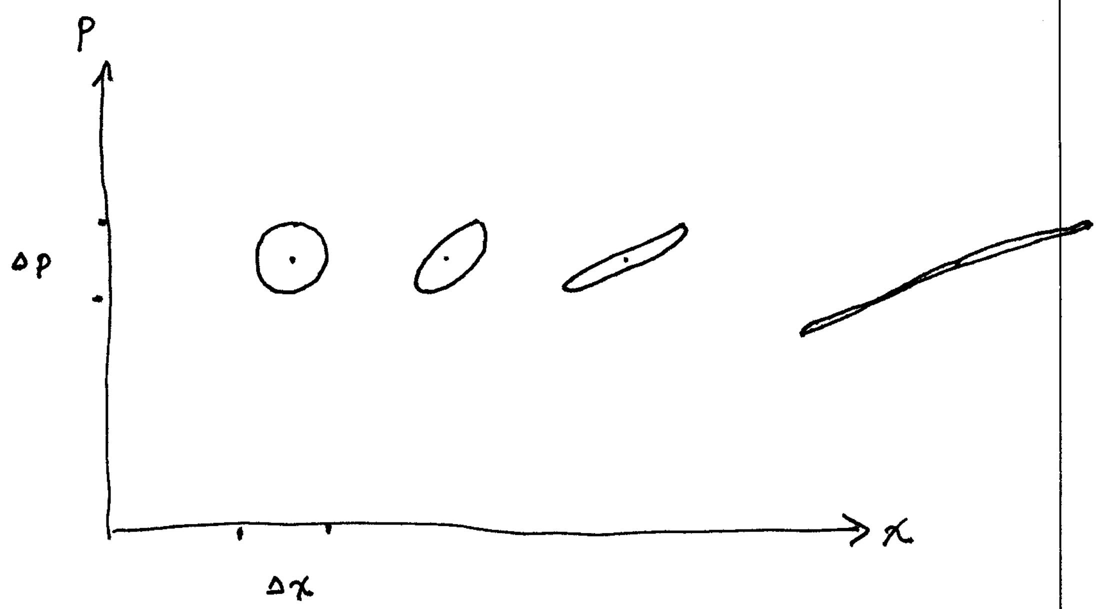
CLASSICAL SPREAD

$\Delta x(t) = \Delta v\, t$

NOT TO SCALE!



CLASSICAL PHASE SPACE



Chapter 1: The Math
Chapter 2: The Postulates

One-dimensional problems

Many 3d problems, for example the hydrogen atom, can be decomposed into a 1d problem in the radial direction coupled to a 2d problem in the theta and phi directions.

Chapter 4: Scattering in 1d

Free particle eigenstates in 1d
Transmission and reflection coefficients

Chapter 5: The infinite square well

Bound particle states in 1d

Chapter 3: Gaussian wave packets

Finite extent free particle states in 1d
The spreading of 1d wavepackets

Chapter 8: The simple harmonic oscillator

Gaussian bound states in 1d

LECTURE 18 JULY 23, 2007

SOLVE SHO DIFF EQ

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

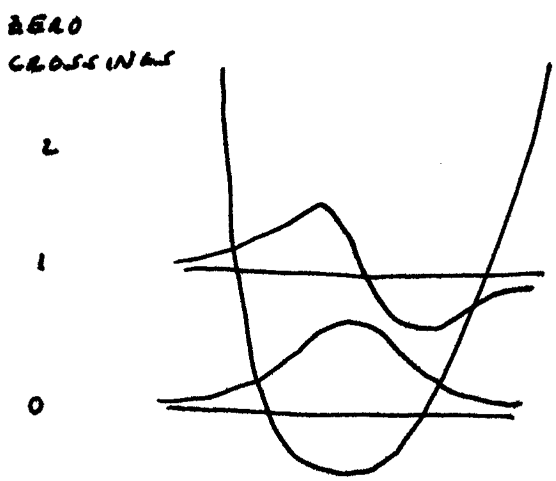
to get x-space, dot with $\langle x |$ bra

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

Find ev's E_n

Find ef's $\varphi_n(x)$

TELL 'EM WHAT YOU'RE GONNA TELL 'EM



FIND ASYPTOTIC FORM OUTSIDE

= GAUSSIAN

SOLUTION = GAUSSIAN X POLYNOMIALS

HERMITE POLYNOMIALS

Lecture 11

SOLVE TISE IN POSITION SPACE

$$H|n\rangle = E_n |n\rangle$$

OPERATOR IN X-SPACE

EIGENENERGIES

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

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

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

STATIONARY STATES

AKA

ENERGY EIGENFUNCTIONS

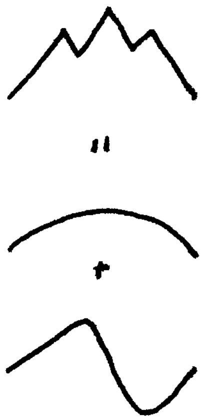
HERMITE POLYNOMIALS

GAUSSIAN

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

SQUARE WELL

INTERVAL:

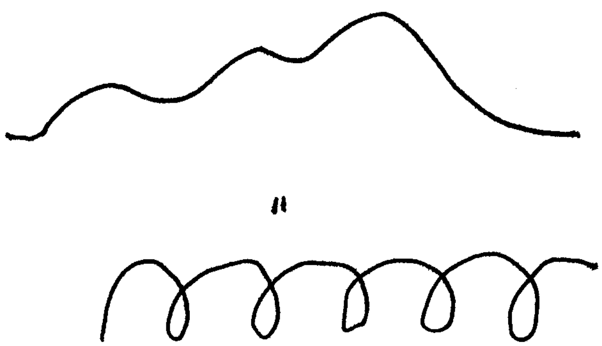


ANY FUNCTION

FOURIER SERIES

$$\psi(x) = \sum_n a_n e^{i k_n x}$$

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

LINE: HERMITE FUNCTIONS

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

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

HYDROGEN ATOM

HALF-LINE

LAGUERRE POLYNOMIALS

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

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

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

SO WE FIRST SOLVE TISE

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

THEN USE

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

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

SO, TO SOLVE TISE...

LECTURE 11: SHO II

POWER SERIES, DIFF EQ'S, AND ALL THAT

TISE

$$H \mid \varphi_n \rangle = E_n \mid \varphi_n \rangle$$

using position basis:

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

OUR JOB: FIND φ_n'S

FIND E_n'S

REWRITE TISE

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

$$\lambda = \frac{2 m E}{\hbar^2}$$

$$\alpha = \frac{m K}{\hbar^2}$$

FIRST STEP: FIND ASYMPTOTIC SOLUTION

FOR LARGE x, $\alpha^2 x^2 >> \lambda$

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

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

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

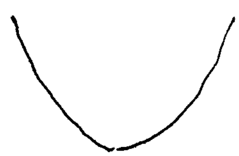
$$\frac{d^2\psi}{dx^2} = \alpha^2 x^2 \; A e^{-1/2\,\alpha x^2} + \alpha^2 x^2 \; B e^{+1/2\,\alpha x^2}$$

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

$\alpha^2 x^2 >> \alpha$

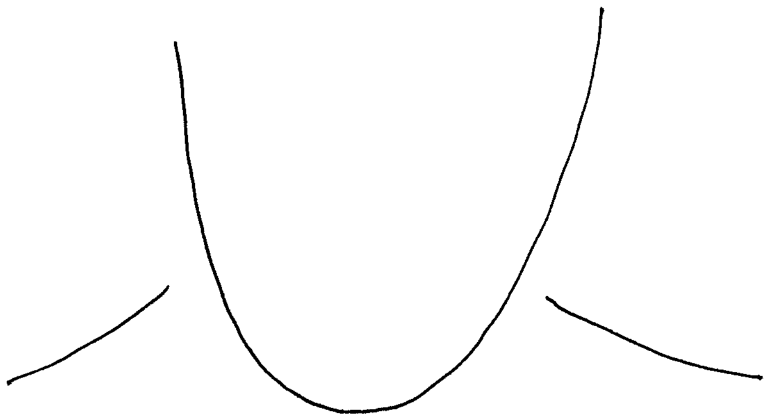
$$\psi(x) = A e^{-\frac{1}{2}\alpha x^2}$$

$$\psi(x) = B e^{+1/2\,\alpha x^2}$$



not square integ

SO, AT LARGE x, WE HAVE GAUSSIAN DECAY



LOOK FOR SOLUTIONS OF THE FORM

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

HERMITE'S EQN

SOLVE USING POWER SERIES...

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

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

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

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

$\Delta m = 2$ $\quad a_0 \Rightarrow$ 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 $\lambda \Rightarrow$ FINITE POLYNOMIALS

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

$\Rightarrow$ EIGENENERGIES!

TWO CLASSES OF SOLUTIONS

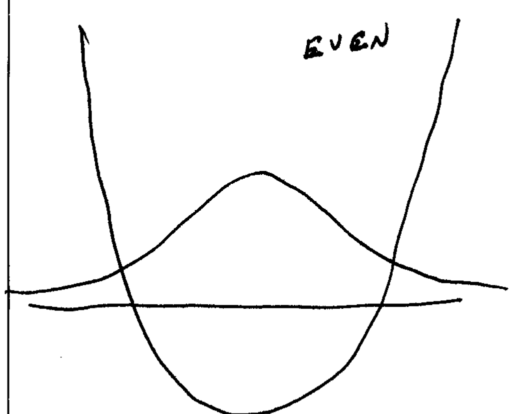
EVEN

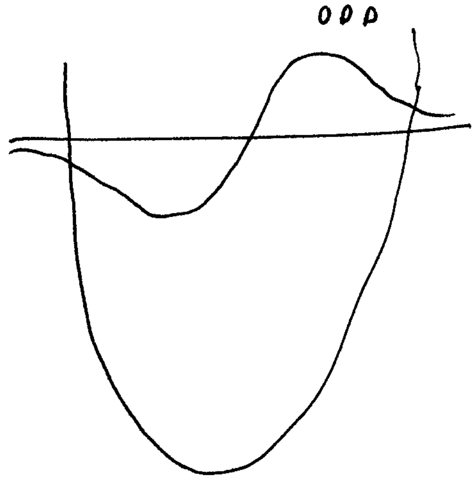
$$H(\xi) = a_0 + a_2 \xi^2 + a_4 \xi^4 + \dots$$

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

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

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

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

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

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

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

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

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

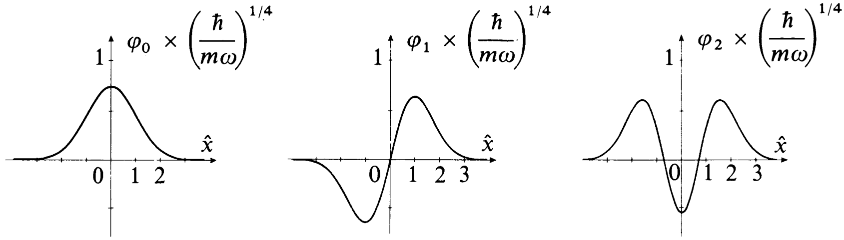


FIGURE 4

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

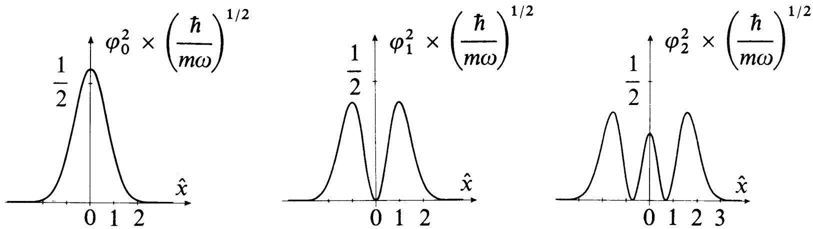


FIGURE 5

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

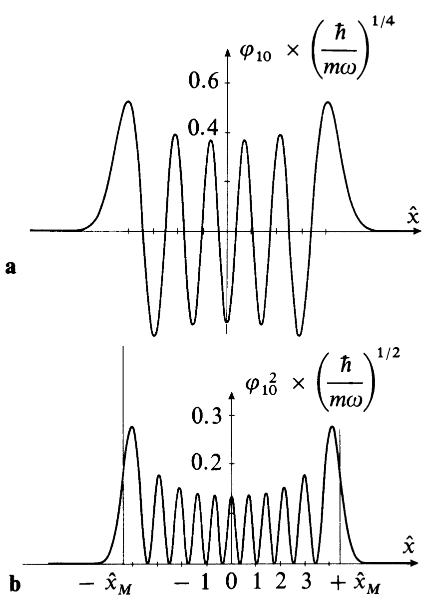


FIGURE 6

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