Lecture 10

The time evolution of arbitrary states
(1) in the square well
(2) in free space

The time evolution of the Gaussian packet in free space

Dispersion

http://www.csupomona.edu/~ajm/materials/animations/packets.html

http://paws.kettering.edu/~drussell/Demos/Dispersion/dispersion.html

Packets

http://webphysics.davidson.edu/Applets/QTime/QTime_Examples.html

http://msc.phys.rug.nl/QuantumMechanics/potential.htm

Superluminal

http://gregegan.customer.netspace.net.au/APPLETS/20/20.html

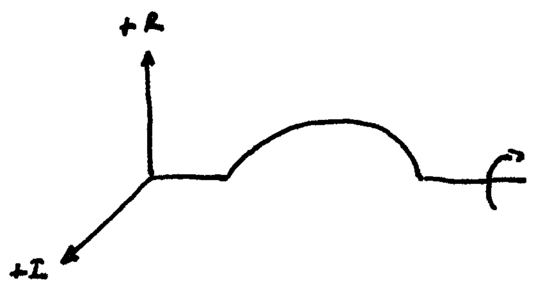
TIME-DEPENDENCE OF THE ENERGY EIGENKETS

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

TIME-DEPENDENCE OF THE STATIONARY STATES

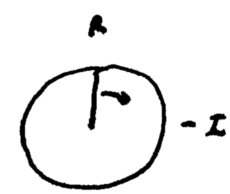
$$\psi_n(x,t) = e^{-iE_nt/\hbar}\,\psi_n(x)$$

IN POSITION SPACE



$\omega_1 = E_1/\hbar$

CLOCK HAND

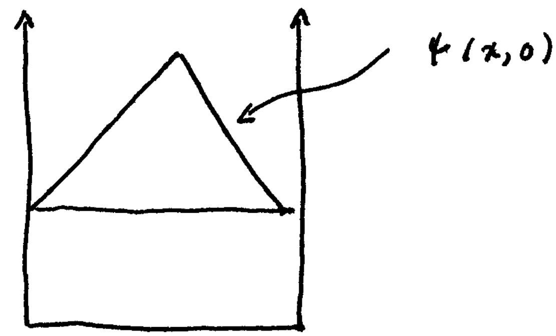


$\omega_2 = E_2/\hbar = 4E_1/\hbar$

$\omega_2 = 4\omega_1$

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

TIME-DEPENDENCE OF AN ARBITRARY STATE



FOUR-STEP PLAN

(1) DIAGONALIZE H

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

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

(4) CALCULATE EVERYTHING $\langle x\rangle$ Δx

$\langle p\rangle$ Δp

$\langle E\rangle$ ΔE

$\vdots$

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

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

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

in x basis

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

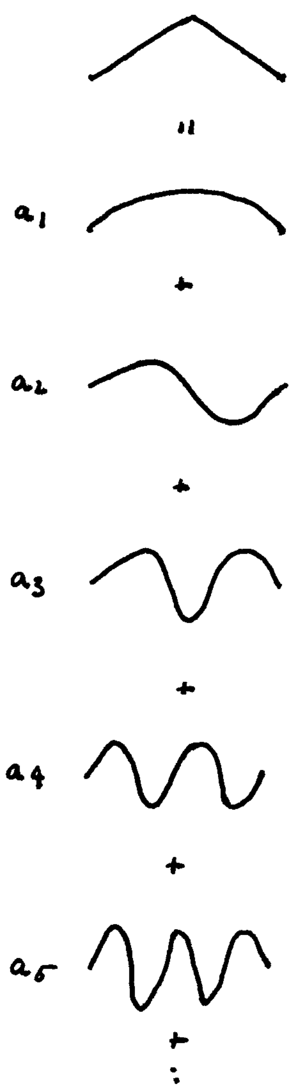
EXPANSION COEFFICIENTS

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

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

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

CARTOON VERSION



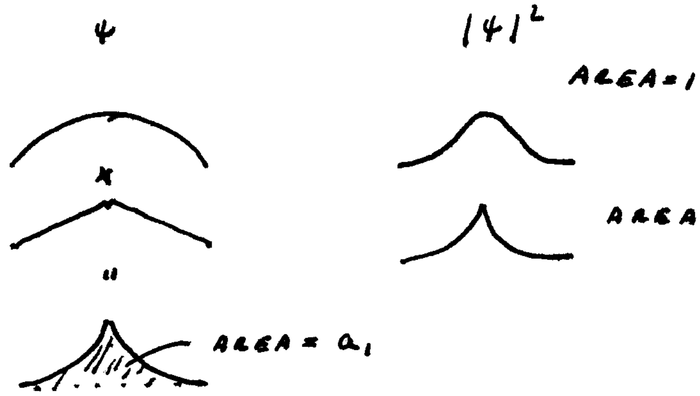
SYMMETRY => ONLY ODD TERMS

TO CALCULATE THE EXPANSION COEFFS

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

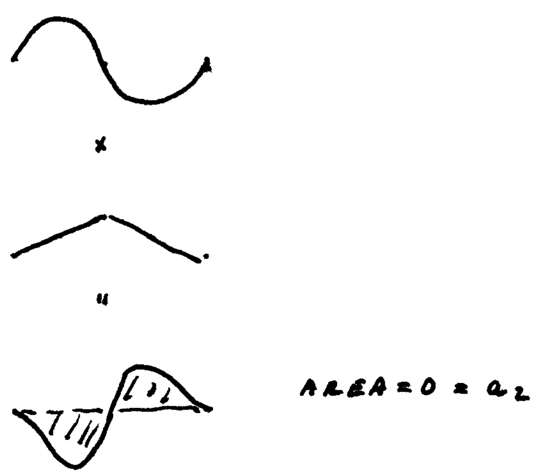
$$= \int_0^L \sqrt{\frac{2}{L}}\ \sin\left(\frac{n\pi}{L}x\right)\ \psi(x,0)\ dx$$

a_1



called overlap integrals

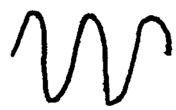
a_2



TIME - DEPENDENCE

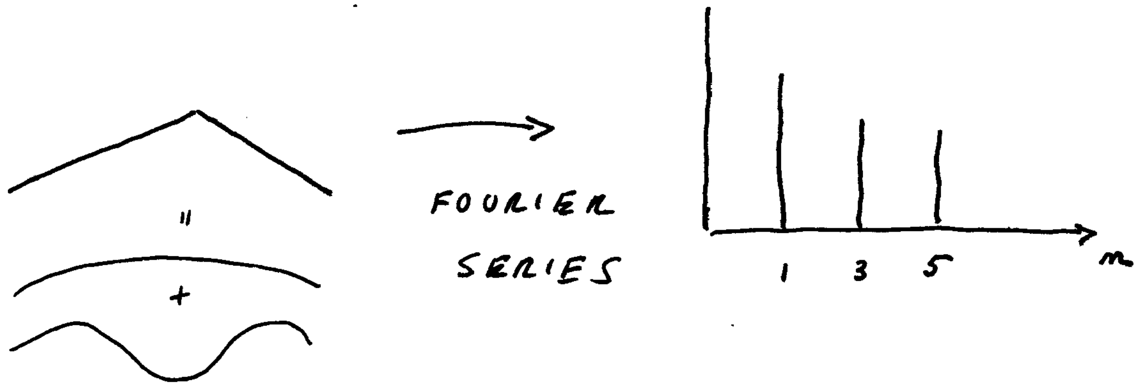
$\psi(x,t) = \quad a_1 e^{-i\omega_1 t}$  T_1

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

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

$\Rightarrow$ RECURRENCE TIME $= T_1$!

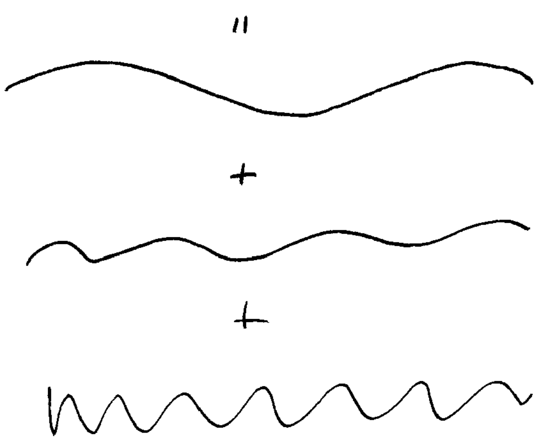
FOR THE SQUARE WELL



a_n's are the FOURIER SERIES EXPANSION COEFFS! DISCRETE

FOR THE FREE PARTICLE

Gaussian



a_n's are given by the Fourier transform coeffs

CONTINUOUS

SHOW MOVIES HERE!?

EIGENSTATES FOR THE FREE PARTICLE

$$\Psi(x,t) \quad A\, e^{\pm i k x}\, e^{-i E_k t/\hbar}$$

$$E_k = \frac{\hbar^2 k^2}{2m} \qquad E_p = \frac{p^2}{2m}$$

$|E\rangle$ ARE 2-FOLD DEGENERATE

$$|\Psi\rangle = \alpha\,|+p\rangle + \beta\,|-p\rangle$$

MEASURE MOMENTUM

$+p \qquad |\alpha|^2$

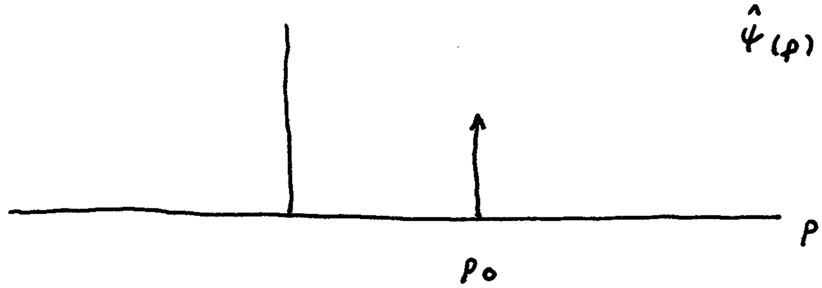
$-p \qquad |\beta|^2$

MEASURE ENERGY

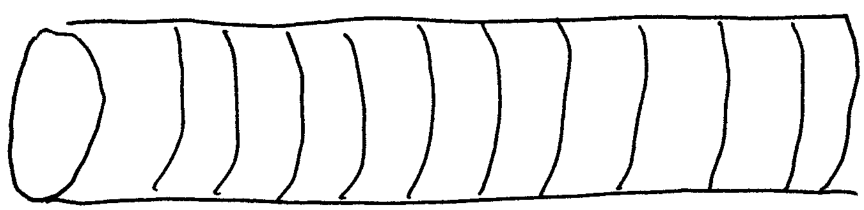
$E = \dfrac{p^2}{2m}$ 100% of the time

IN MOMENTUM SPACE

$$\hat{\psi}(p) = \delta(p - p_0)$$



IN X-SPACE $\quad \psi(x) = e^{i p_0 x/\hbar} = e^{i k_0 x}$



RH HELIX

PITCH = K_0 SPATIAL WAVELENGTH

EIGENSTATE OF p : "INFINITE PLANE WAVE"

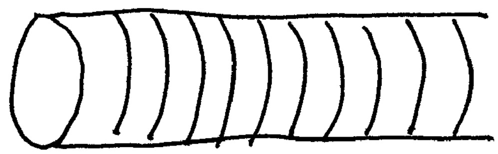
PLANE WAVE OF INFINITE SPATIAL EXTENT

EIGENSTATE OF E : PLANE WAVE WITH INFINITE TEMPORAL EXTENT

OBVIOUSLY IDEALIZATIONS!

FREE WAVE PACKETS

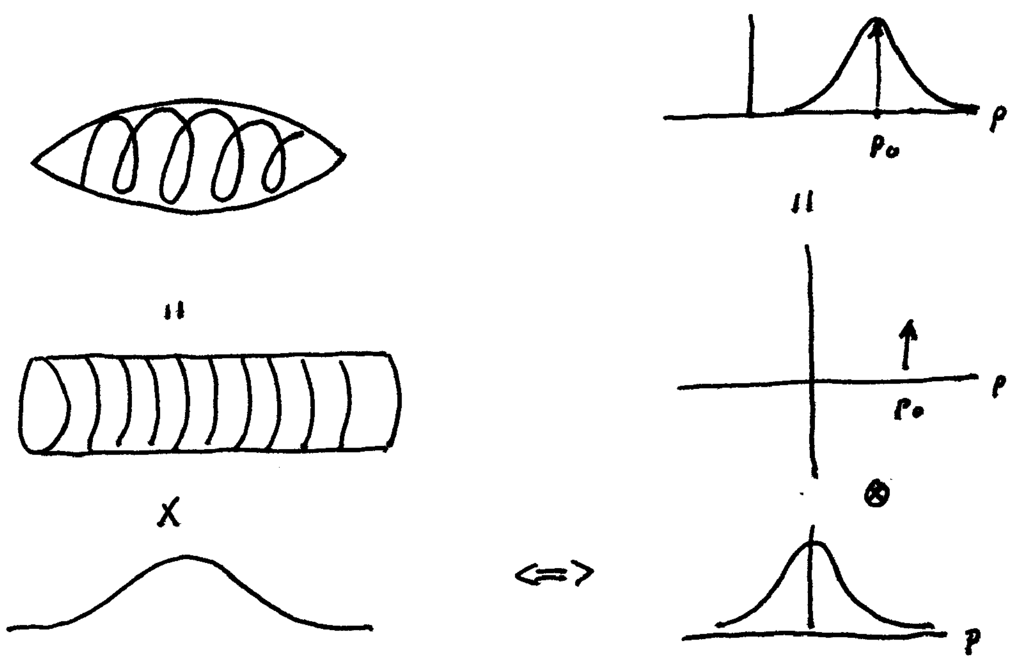
PLANE WAVE $e^{ip_0 x/\hbar}$



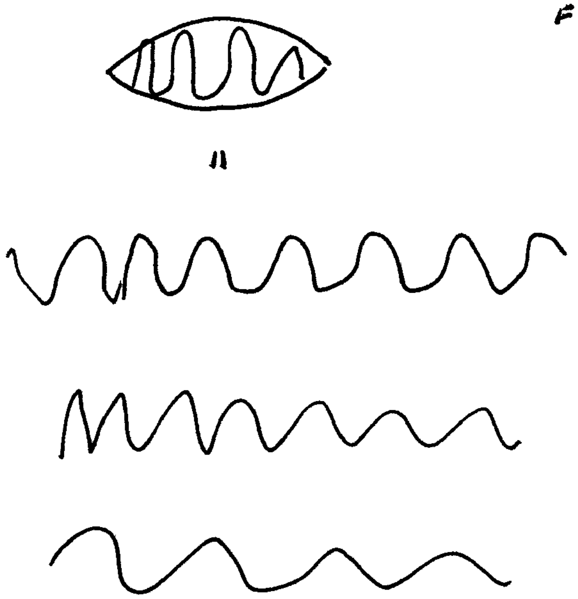
INFINITE EXTENT $\Rightarrow$ $\Delta X = \infty$

$$\Delta x \, \Delta p \geq \frac{\hbar}{2} \Rightarrow \Delta p = 0$$

an idealization since the universe is finite



SPREADING OF THE WAVEPACKET



FINITE PACKET

FT

INTEGRAL OVER INFINITE EXTENT WAVES

if component waves move at the same velocity, then ~~waves~~ packet stays together

LIGHT IN VACUUM

if component waves move with different velocities, then packet disperses

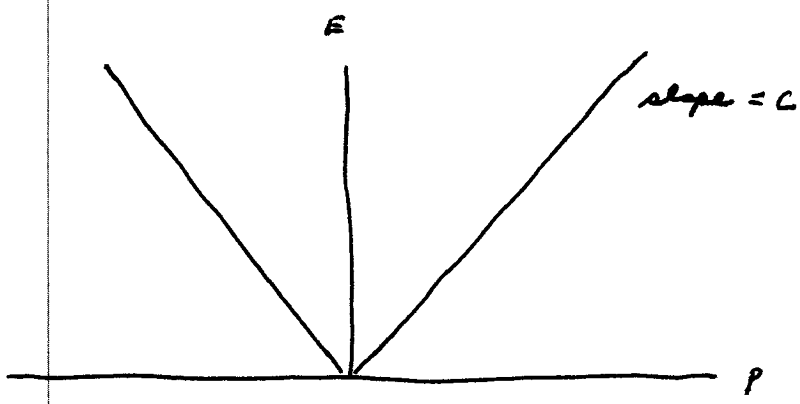
LIGHT IN A PRISM

ELECTRONS IN A VACUUM

EMPTY SPACE IS DISPERSIVE FOR MATTER WAVES

" " " NON- " " EM WAVES

LIGHT $\quad E = pc \quad$ LINEAR

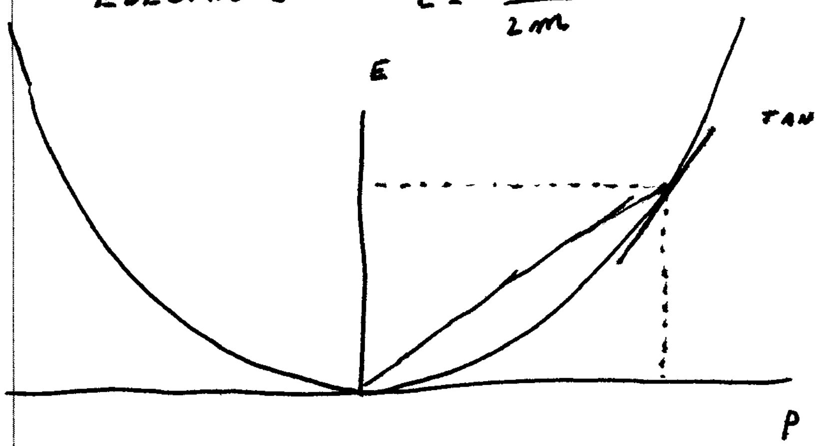


$E(p) \qquad E = \hbar\omega \qquad p = \hbar k$

$\omega(k)$

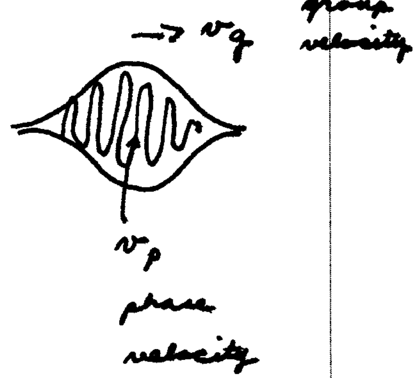
FUNCTIONS are called dispersion relation

ELECTRONS $\quad E = \dfrac{p^2}{2m} \quad$ PARABOLIC



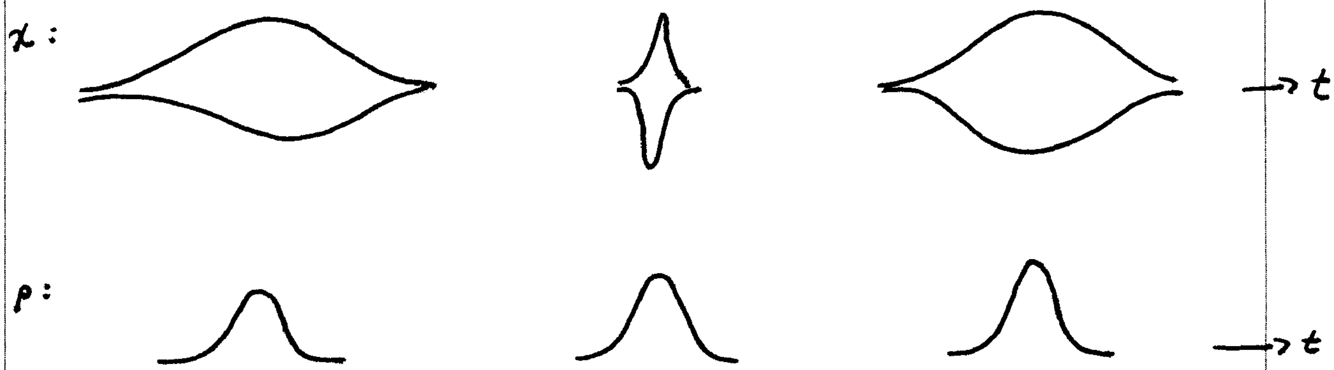
TANGENT LINE

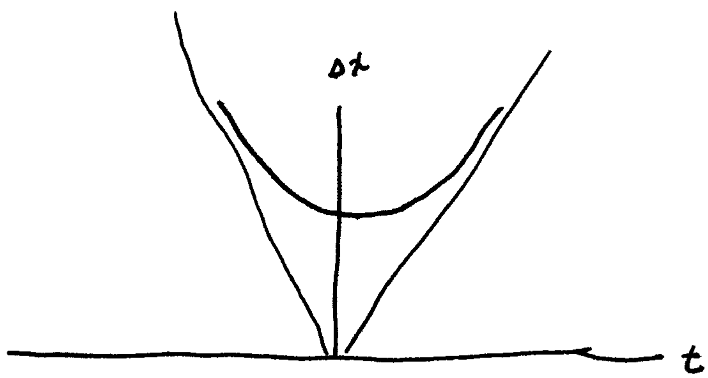
$$\text{slope} = \frac{dE}{dp} = \frac{2p}{2m} = v$$

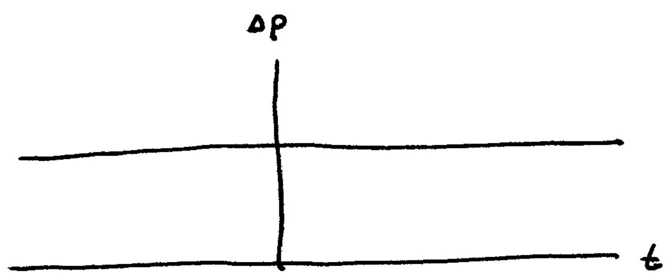


CHORD

$$\text{slope} = \frac{E}{p} = \frac{\frac{p^2}{2m}}{p} = \frac{1}{2}\,\frac{p}{m} = \frac{1}{2}\,v$$


x:
p:
t
t


Δx
t


Δp
t

(1) FINISH FREE WAVE PACKET

QUANTITATIVE

(2) START HARMONIC OSCILLATOR

$$\psi(x,0) = e^{i p_0 x/\hbar} \quad (\pi^{*}\Delta^2)^{-1/4} \quad e^{-x^2/2\Delta^2}$$

PLANE WAVE | GAUSSIAN ENVELOPE

$\langle p \rangle = p_0$ | $\langle x \rangle = 0$

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

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

MINIMUM UNCERTAINY AT $t = 0$

INCLUDE THE TIME-DEPENDENT PHASE FACTORS

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

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

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

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

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

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

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

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

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

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

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

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

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

GAUSSIAN
ENVELOPE

MIN WIDTH => $\Delta X = \dfrac{\Delta}{\sqrt{2}}$

TIME-DEPENDENT WIDTH

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

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

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

$\sim \dfrac{t}{\Delta}$ SMALLER D => FASTER SPREAT

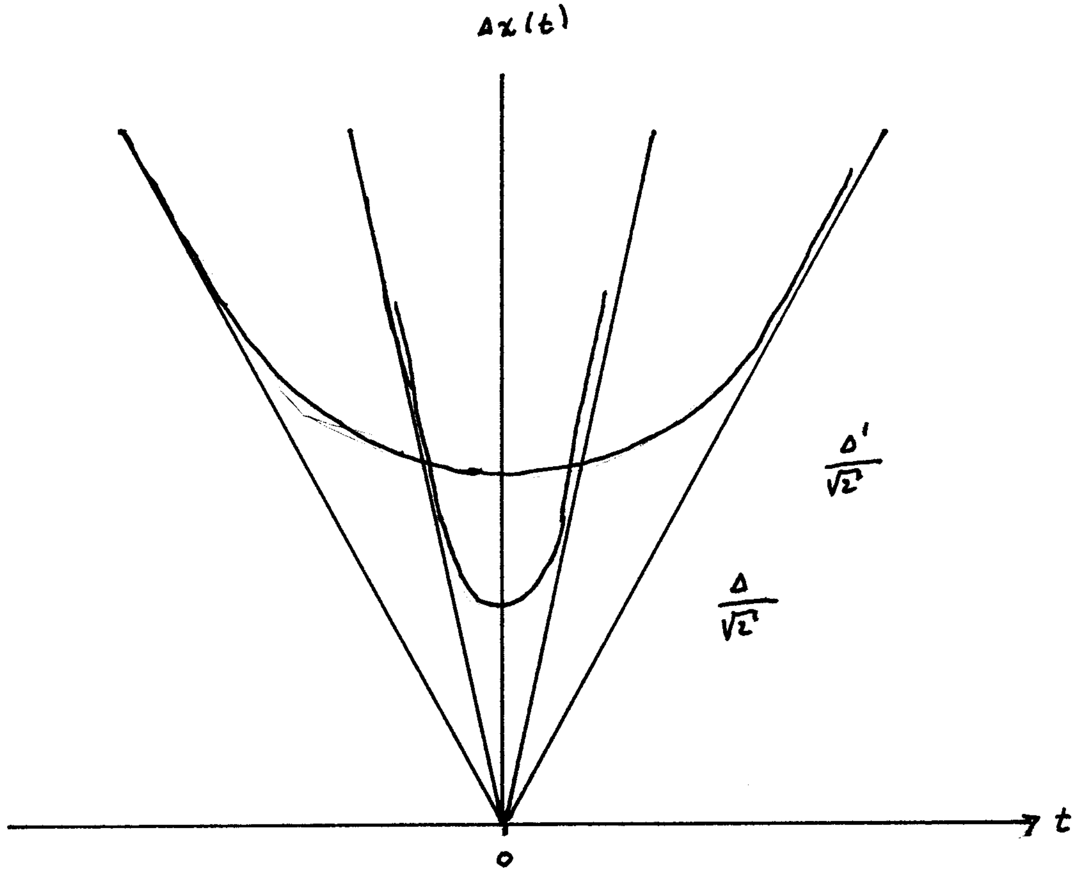
$\Delta p(t) = \dfrac{\hbar}{\sqrt{2}\, \Delta}$ CONSTANT

$\Delta v = \dfrac{\hbar}{\sqrt{2}\, m \Delta}$ SMALLER Δ => LARGE Δv

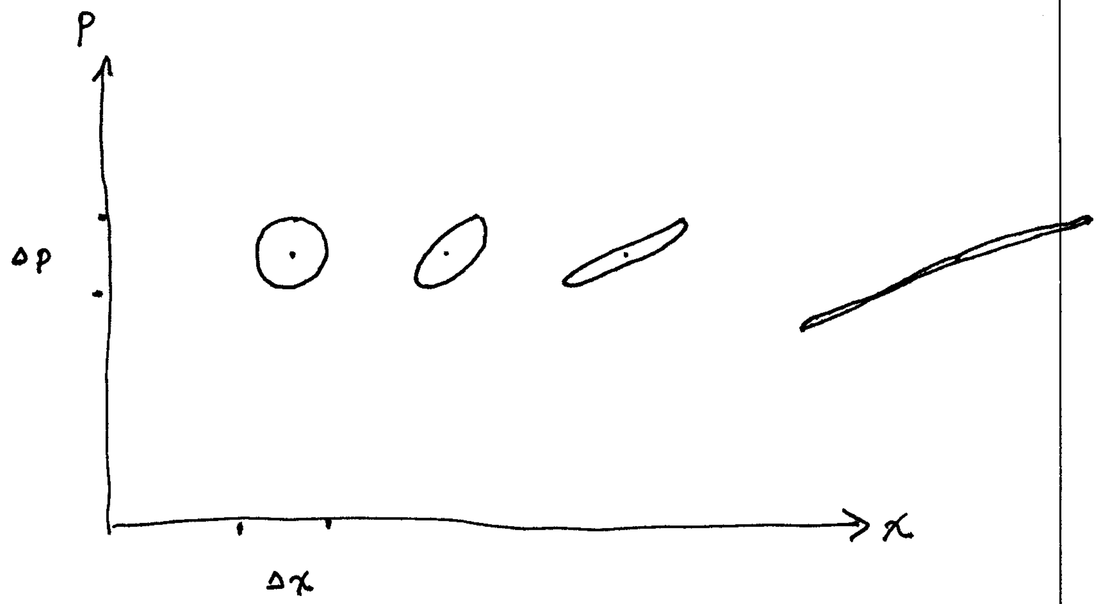
CLASSICAL SPREAD

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

NOT TO SCALE!



CLASSICAL PHASE SPACE



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

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

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

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

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

$$\psi(x,t)=\int U(x,t;x',t')\psi(x',t')\,dx'\qquad(5.1.12)$$

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

$$\psi(x', 0) = e^{ip_0 x'/\hbar} \frac{e^{-x'^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}} \tag{5.1.14}$$

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

$$\begin{aligned}\psi(x, t) = \left[\pi^{1/2}\left(\Delta + \frac{i\hbar t}{m\Delta}\right)\right]^{-1/2} \cdot \exp\left[\frac{-(x - p_0 t/m)^2}{2\Delta^2(1 + i\hbar t/m\Delta^2)}\right] \\ \times \exp\left[\frac{ip_0}{\hbar}\left(x - \frac{p_0 t}{2m}\right)\right]\end{aligned} \tag{5.1.15}$$

The corresponding probability density is

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

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

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