Chapter 3

Formalism

Hilbert Space

Two kinds of mathematical constructs

- wavefunctions (representing the system)
- operators (representing observables)

Vector

Consider a *N*-dimensional vector wrp to a specific orthornormal basis $\{|\hat{e}\rangle\}$

$$|\alpha\rangle = |a_1, a_2, a_3, ..., a_N\rangle$$

Inner project of two vectors

$$\langle \alpha | \beta \rangle = a_1^* b_1 + a_2^* b_2 + \dots + a_N^* b_N$$

Functions, as vectors

A function is a vector with infinite dimensionality. Example:

$$f(x) = \sum_{n=0}^{n=\infty} a_n \cos(n\pi x) + b_n \sin(n\pi x)$$

$$f(x) = \{a_{1,}a_{2,..};b_{1,}b_{2,...}\}$$
 in the basis
$$\{\cos n\pi x; \sin n\pi x\}$$

Functions, as vectors

A function is a vector with infinite dimensionality. Example:

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Wave function

A wave function in QM has to be normalised,

$$\int |\Psi|^2 dx = 1.$$

Hence, in QM, we consider only the collection of all function that are square integrable

$$f(x)$$
 such that $\int |f(x)|^2 dx < \infty$

Hilbert space

The collection of all square integrable functions constitute a Hilbert space, which is a subset of the vector space.

Wave functions live in Hilbert space.

All functions living in Hilbert space is square integrable

Inner product

Since all functions living in Hilbert space is square integrable, the inner product of two functions in the Hilbert space is guaranteed to exist

$$\langle f|g\rangle \equiv \int_a^b f(x)^* g(x) dx$$

By definition of the inner product

Take the complex conjugate of the inner product, you will get

$$\langle f|g\rangle \equiv \int_a^b f(x)^* g(x) dx$$

Complex conjugate

$$\langle f|g\rangle^* \equiv \int_a^b f(x) \ g(x) dx = \langle g|f\rangle$$

"permuting the order in the inner product amounts to complex conjugating it."

Inner product of the same function

$$\langle f|f\rangle = \int_{a}^{b} |f(x)|^{2} dx$$

real and non-negative

Schwarz inequality

$$\left| \int_{a}^{b} f(x)^{*} g(x) dx \right| \leq \sqrt{\int_{a}^{b} |f(x)|^{2}} dx \int_{a}^{b} |g(x)|^{2} dx$$

$$|\langle f|g\rangle|^2 \le \langle f|f\rangle\langle g|g\rangle$$

The only function whose inner product with itself vanishes is 0, i.e.

$$\langle f|f\rangle = 0 \Rightarrow f(x) = 0$$

Orthogonality

Two functions are said to be orthogonal if

$$\langle g|f\rangle = 0$$

A set of functions, $\{f_n\}$, is orthornomal if they are normalised and mutually orthornomal:

$$\langle f_n | f_m \rangle = \delta_{mn}$$

Completeness

A set of functions is complete if any other function (in Hilbert space) can be expressed as a linear combination of them:

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$$

Making sense of these definitions

Try to make sense of these definitions by making contact with what you have learned in the previous chapters

The stationary states for the infinite square well constitute a complete orthonomal set on the interval (0, *a*);

The stationary states for the harmonic oscillator are a complete set on the interval $(-\infty, +\infty)$.

Expectation value of an observable in terms of inner product

$$\langle Q \rangle = \int \Psi^* \hat{Q} \Psi dx = \langle \Psi | \hat{Q} \Psi \rangle$$

The observable has to be a real number, and it is the average of many measurement:

$$\langle Q \rangle = \langle Q \rangle^*$$

Such mathematical requirement results in the fact that not any operator can be a valid observable in QM.

To be a valid observable in QM, an operator must obey the requirement

$$\langle Q \rangle = \langle Q \rangle^*$$

$$\Rightarrow \langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle$$

This can be proven by using the fact that

$$\langle f|g\rangle^* = \langle g|f\rangle$$

Proof

$$Given \langle Q \rangle = \langle Q \rangle^*$$
 $\langle \Psi | Q\Psi \rangle = \langle \Psi | Q\Psi \rangle^*$
 $But \langle \Psi | Q\Psi \rangle^* = \langle Q\Psi | \Psi \rangle$
 $Therefore,$
 $\langle \Psi | Q\Psi \rangle = \langle Q\Psi | \Psi \rangle$

Hermitian operator

The operators representing observable in QM, Q, has the property that

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle$$

for all f(x), g(x)

Such operators are called Hermitian.

Hermitian operator arises naturally in QM because their expectation values are real.

Why Hermitian operators?

Observables in QM are represented by Hermitian operators \hat{Q}

Fourier's trick to project out the coefficients

If the functions $\{f_n(x)\}\$ are orthornomal,

$$c_n = \langle f_n | f \rangle$$

Adjoin / Hermitian conjugate

The adjoin or the conjugate of a Hermitian operator is defined as

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}^{\dagger}f|g\rangle$$

for all f and g.

Q a Hermitian operator

 Q^{\dagger} adjoin to Q

In general, a Hermitian operator is equal to its conjugate, i.e.,

$$\hat{Q}^{\dagger} = \hat{Q}$$

$$\hat{p}^{\dagger} = \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$
, and $\hat{x}^{\dagger} = \hat{x}$.

Example

Show that
$$\hat{p}^{\dagger} = \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$
 (i.e., the momentum operator is Hermitian)

For this purpose, you need to show that

$$\langle f|\hat{p}g\rangle = \int_{-\infty}^{\infty} f^* \frac{\hbar}{i} \frac{dg}{dx} dx = \dots = \langle \hat{p}f|g\rangle$$

Hint: you need to use integration by parts

Determinant states

• An determinate state for an observable *Q* is one in which every measurement of *Q* is certain to return the same value.

Example:

Stationary states are determinate state of the Hamiltonian H (which is the observable energy).

A measurement of the total energy on a particle in the stationary state Ψ_n is certain to yield the corresponding allowed energy E_n .

The variance of Q in a determinate state is zero

$$\sigma^{2} = \langle (\hat{Q} - \langle Q \rangle)^{2} \rangle$$

$$= \langle \Psi | (\hat{Q} - q)^{2} \Psi \rangle$$

$$= \langle (\hat{Q} - q) \Psi | (\hat{Q} - q) \Psi \rangle = 0$$

$$\hat{Q} \Psi = q \Psi$$

This is an eigenvalue equation for the operator Q

In QM, determinate states of Q are known as "eigenfunctions of Q"

$$Q\Psi = q\Psi$$

 Ψ is an eigenfunction of Q, and q is the corresponding eigenvalue.

To sum up

If a system is in a state Ψ that is a determinate state of operator Q, then:

- 1)Every time a measurement is made for the observable Q, the system in the state Ψ will always return a same measured value q as a result of the measurement.
- 2) The mathematical description of a determinate state is provided by the eigenvalue equation,
- $\Psi = q\Psi$ is known as an eigenfunction of Q; q the corresponding eigenvalue.

Spectrum

An observable Q in an eigenvalue equation has a set of eigenvalues, $\{q_1, q_2, q_3,,\}$

The collection of all the eigenvalues of an operator is called its spectrum.

Example:
$$\hat{H}\psi_n = E_n\psi$$

The spectrum are the set of discrete eigenenergies $\{E_n\}$

Degeneracy

Sometimes two distinct eigenfunctions may share a same eigenvalue,

$$H\Psi_{1} = \epsilon \Psi_{1}$$

$$H\Psi_{2} = \epsilon \Psi_{2}$$

$$\Psi_{1} \neq \Psi_{2}$$

The spectrum is said to be degenerate for the states Ψ_{1} , Ψ_{2}

Eigenfunctions and eigenvalues are intrinsic to an operator $Q\Psi = q\Psi$

Given a Hermitian operator \hat{Q} there always exist a set of eigenfunctions and the corresponding eigenvalues.

In QM, the major task is to find out what are the engenfunctions and the corresponding eigenevalues of that operator.

Why you need to solve the eigenvalue problem of Q?

$$Q\Psi = q\Psi$$

We need to find out the eigenvalues and eigenfunctions of a Hermitian operator Q because ...

These eigenvalues and eigenfunctions are the determinate states that form the stationary solutions to the Schroedinger Equation.

Solving the eigenvalue problem of the corresponding Hermitian operator is an integral part to the total prediction of the related observable in QM.

Example:
$$\hat{Q} \equiv i \frac{d}{d\phi}$$

 ϕ is the usual polar coordinate in 2D

Is \hat{Q} hermitian?

Find its eigenfunctions and eigenvalues.

Q is a hermiatian because

$$\langle f | \hat{Q} g \rangle = \int_0^{2\pi} f^* \left(i \frac{dg}{d\phi} \right) d\phi = \dots = \langle \hat{Q} f | g \rangle.$$

Show this.

Solving the eigenvalue problem for

$$\hat{Q} \equiv i \frac{d}{d\phi}$$

$$i\frac{d}{d\phi}f(\phi) = qf(\phi)$$

 $i\frac{d}{d\phi}f(\phi)=qf(\phi)$ We want to know what the function $f(\phi)$ looks like

Due to the definition ϕ as the polar angle of a quantum system, cyclic boundary condition is to be imposed on $f(\phi)$:

$$f(\phi)=f(\phi+2\pi)$$

Solving the eigenvalue problem

$$i\frac{d}{d\phi}f(\phi) = qf(\phi)$$

Solution:

$$f(\phi) = Ae^{-iq\phi}$$

Due to periodic boundary condition in ϕ , $f(\phi)=f(\phi+2\pi)$ The possible values of the q is restricted to

$$q = 0, \pm 1, \pm 2, \dots$$

Prove this.

The spectrum of this operator is the set of all integers, and it is nondegenerate

Checkpoint questions

Consider a particle in an infinite quantum well where the wavefunction of the particle is given by the ground state Ψ_0 .

Is the particle an determinate state of the position operator?

Is the particle an determinate state of the Hamiltonian operator?

Two categories of Hermitian operators

- 1. With discrete spectrum (e.g., Hamiltonian for harmonic oscillator, Hamiltonian for infinite square well, etc.)
- Those eigenfunctions with with discrete eigenvalues are normalisable and live in Hilbert space. They represents physically realisable states.

- 2. With continuous spectrum (e.g., Hamiltonian for free particle)
- Eigenfunctions with continuous eigenvalues are not normalisable, hence do not represents physically realisable states.

Mathematical properties of normalisable eigenfunctions of a Hermitian operator

(1) Reality: Their eigenvalues are real

$$\hat{Q}f = qf$$
, then $q = q^*$

Proof:

$$\hat{Q}f = qf$$
 \hat{Q} is hermitian

$$\langle f|\hat{Q}f\rangle = \langle \hat{Q}f|f\rangle$$

$$\langle f|\hat{Q}f\rangle = \langle f|qf\rangle = \int f(x)(qf(x))dx = q \int f(x)f(x)dx = q \langle f|f\rangle$$

$$\langle \hat{Q}f|f\rangle = \langle qf|f\rangle = \int (qf(x))^* f(x)dx = q^* \int f(x)f(x)dx = q \langle f|f\rangle$$

$$\Rightarrow q = q^{\hat{}}$$

Mathematical properties of normalisable eigenfunctions of a Hermitian operator

(2) Orthogonality: Eigenfunctions belonging to distinct eigenvalues are orthogonal.

$$\hat{Q}g = q'g, \hat{Q}f = qf.$$

If
$$q \neq q'$$
, then $\langle f|g\rangle = 0$

This is useful so that we can apply Fourier's trick

Proof of orthogonality

Orthogonality: Eigenfunctions belonging to distinct eigenvalues are orthogonal.

Proof:

$$\hat{Q}g = q'g, \hat{Q}f = qf$$

$$\begin{vmatrix} \hat{Q} & \text{is hermitian} \\ \langle f|\hat{Q}g \rangle = \langle \hat{Q}f|g \rangle \end{vmatrix}$$

For the statement to be true,

$$q' < f \mid g > = q < f \mid g >; q \neq q'$$

 $< f \mid g > = 0$ whenever $q \neq q' \longrightarrow$ This is orthogonality

Orthogonality, stated in a different way

 $< f \mid g> = 0$ whenever $q \neq q'$

This is just the orthogonality condition on the stationary solutions we have seen in Chapter 2 (but stated in a more rigorous way)

Mathematical properties of normalisable eigenfunctions of a Hermitian operator

(3) Completeness: The eigenfunctions of an observable operator are complete: Any function in Hilbert space can be expressed as linear combination of them.

Recall that you have seen these three properties in the stationary solutions in Chapter 2!!!

$$f(x) = \sum c_n f_n(x)$$

 $\{f_n(x)\}\$ the set of eigenfunctions living in Hilbert space (hence normalisable)

Hermitian operator with continuous spectrum

The three mathematical properties for the eigenfunctions with discrete eigenvalues are "desirable" properties for QM.

We wish that these would have also happened to Hermitian operators with continuous spectrum.

Eigenfunction of Hertmitian operators with continuous spectra are not normalisable

- Specific example of Hermitian operator with continuous spectrum: momentum, position operator for free particle.
- This case is slightly complicated compared to the case with discrete spectra as the eigenfunctions are not normalisable.
- This is because the inner products may not exist.
- However, reality, orthorgonality and completeness of the eigenfunctions still hold (but manifest themselves in a mathematically different way)

Momentum operator as an example of Hertmitian operators with continuous spectra

$$\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$$

Let $f_p(x)$ and p be the eigenfunction and eigenvalue for \hat{p}

$$\hat{p}f_p(x) = pf_p(x)$$

The general solution is $f_p(x) = Ae^{ipx/\hbar}$

$$\langle f_p | f_{p'} \rangle = \int_{-\infty}^{\infty} f^*_{p'}(x) f_p(x) dx = |A|^2 \int_{-\infty}^{\infty} e^{i(p-p'^*)x/\hbar} dx$$

This is not square-integrable for a generic value (complex in general) of p,

Note: If p is complex, $p \neq p^*$

Restoring orthogonality

However, orthogonality of the eigenfunction can be restored if we restrict only to real values of the eigenvalues p (i.e., $p^* = p$):

Rewrite the inner product of the eigenfunctions as

$$\langle f_p | f_{p'} \rangle =$$

$$\int_{-\infty}^{\infty} f^*_{p'}(x) f_p(x) dx = |A|^2 \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar} dx$$

Dirac delta function in integral form (1)

Plancherels theorem, we can express Dirac delta function $\delta(x)$ in terms of its fourier transform F(k):

$$\delta(x) = \frac{1}{\sqrt{2\pi}} \int F(k)e^{ikx}dk.$$

$$F(k) = \frac{1}{\sqrt{2\pi}} \int \delta(x) e^{-ikx} dx$$

Dirac delta function in integral form (2)

$$F(k) = \frac{1}{\sqrt{2\pi}} \int \delta(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}}$$

This is the result of the definition of the Dirac delta function,

$$\int \delta(x)f(x)dx = f(0)$$

$$\delta(x) = \frac{1}{\sqrt{2\pi}} \int F(k)e^{ikx}dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx}dk$$

$$\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x - x')}dk$$

$$\int_{-\infty}^{\infty} e^{i(p' - p)y}dy = 2\pi\delta(p' - p)$$
Show this

"Dirac orthonormality"

$$\int_{-\infty}^{\infty} f^*_{p'}(x) f_p(x) dx = |A|^2 \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar} dx$$
$$= |A|^2 2\pi \hbar \delta(p'-p)$$
hereging $A = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar} dx$

Choosing
$$A = \frac{1}{\sqrt{2\pi\hbar}}, \quad \langle f_p | f_{p'} \rangle = \delta(p' - p)$$

"Dirac orthornomalilty"

This is the orthonormality statement for eigenfunctions with continuous spectrum.

To sum up the previous slides

The reality of eigenvalues and orthogonality of the eigenfunctions of the momentum operator, which is an example of Hermitian operator with continuous spectrum, are "restored":

• $p = p^*$ (reality is "imposed")

$$\langle f_p | f_{p'} \rangle = \delta(p' - p)$$

As comparison: reality and orthonormality statements for the normalisable eigenfunctions case are

$$\hat{Q}f = qf$$
, then $q = q^*$
 $\langle f_m | f_n \rangle = \delta_{m,n}$

Check point question

Does $\delta(p - p')$ any different than $\delta(p' - p)$?

Completeness

The eigenfunctions $f_{\rho}(x)$ with continuous, real eigenvalues are complete, in the sense that any square-integrable function f(x) can be written as an integral the form

$$f(x) = \int c(p)f_p(x)dp$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int c(p)e^{ipx/\hbar} dp$$

This is considered as an axiom, which is to be accepted and not to be proven.

Coefficient c(p)

c(p) in the expansion of f(x) can be obtained via Fourier's trick (thanks to Dirac's orthonormality)

$$\begin{split} \langle f_{p'}|f\rangle &= \int_{-\infty}^{\infty} f_{p'}^*(x)f(x)dx \\ &= \int_{-\infty}^{\infty} f_{p'}^*(x) \left\{ \int_{-\infty}^{\infty} c(p)f_p(x)dp \right\} dx \\ &= \int_{-\infty}^{\infty} c(p) \left\{ \int_{-\infty}^{\infty} f_{p'}^*(x)f_p(x)dx \right\} dp \\ &= \int_{-\infty}^{\infty} c(p)\delta(p'-p)dp = c(p') \end{split}$$

Another example of Hermitian operator with continuous spectrum: position operator

Find the eigenvalues and eigenfunctions of the position operator.

$$\hat{x}g_y(x) = yg_y(x)$$

We want to know what is the eigenfunction $g_y(x)$, and the eigenvalue y.

The eigenfunction of the continuous observable *x*

$$\hat{x}g_y(x) = yg_y(x)$$

What is a function of x that has the property that multiplying it by x is the same a multiplying it by a constant y?

The eigenfunction turns out to be

$$g_y(x) = A\delta(y - x)$$

Eigenvalue *y* is real.

 $g_{y}(x)$ is not square integrable, but still Dirac orthonormal (by choosing A = 1):

$$\langle g_{y'}|g_y\rangle = \delta(y-y').$$

The eigenfunction of the continuous observable *x* is complete

$$g_y(x) = A\delta(y-x)$$
 ; A =1

$$f(x) = \int_{-\infty}^{\infty} c(y)g_y(x)dy$$

The coefficient c(x) is trivially given by

$$f(x) = \int_{-\infty}^{\infty} c(y)g_y(x)dy = \cdots$$
$$= \int_{-\infty}^{\infty} c(y)\delta(x - y)dy = c(x)$$

To sum up

If the spectrum of a hermitian operator is *continuous* (so the eigenvalues are labeled by a continuous variable—p or y, in the examples; z, generically, in what follows), the eigenfunctions are not normalizable, they are not in Hilbert space and they do not represent possible physical states; nevertheless, the eigenfunctions with real eigenvalues are Dirac orthonormalizable and complete (with the sum now an integral). Luckily, this is all we really require.

Check-point questions

Is the ground state of infinite quantum well an eigenfunction of momentum?

with
$$n = 1$$
 $\psi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right)$

$$\hat{p}\,\psi_1(x) = \frac{\hbar}{i}\frac{d}{dx}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right) = \dots = \left[-i\frac{\pi\hbar}{a}\cos\left(\frac{\pi}{a}x\right)\right]\psi_1(x)$$

 \neq constant x $\psi_1(x)$.

Hence the ground state $\psi_1(x)$ is not the eigenfunction of momentum operator

Is the ground state of infinite quantum well an eigenfunction of momentum?

What is the magnitude of the momentum in the ground state?

ANS: the magnitude of the momentum is

$$\sqrt{2mE_1} = \pi\hbar/a$$

Since the momentum is definite, why not the ground state a determinate state of the momentum?

ANS: See next slide

Is the ground state of infinite quantum well an eigenfunction of momentum?

ANS: NO. The ground state in the infinite quantum well is not a determinate state of the momentum because it is not the eigenstate of the momentum operator.

The magnitude of momentum is determinate but NOT the direction.

So the fact that the magnitude of the momentum is determinate does not contradict the fact that the ground state is NOT the eigenstate of the momentum operator.

Check point question (easy)

Problem 3.1 (a)

Suppose that f(x) and g(x) are two eigenfunctions of an operator Q, with the same eigenvalue q. Show that any linear combination of f and g is itself an eigenfunction of Q, with eigenvalue q.

Generalised statistical interpretation

QM can't tell you the precise value you will get in a particular measurement (as would be the case in classical mechanics)

In QM, the results of any measurement is not deterministic but "spread out" according to a probability distribution.

How to calculate the possible results of any measurement?

Probability for discrete spectrum

$$\hat{Q}f_n(x) = q_n f_n(x)$$

$$\Psi(x,0) = \sum_{n} c_n f_n(x)$$

 $\{f_n(x)\}\$ are the set of eigenfunctions associated with the operator Q

Probability for discrete spectrum (cont.)

If you measure an observable Q(x, p) on a particle in the state Ψ , you are certain to get one of the eigenvalues of the hermitian operator Q(x, p).

If the spectrum is discrete, the probability of getting the particular eigenvalue q_n associated with the orthornomalised eigenfunction $f_n(x)$ is

$$|c_n|^2$$
, where $c_n = \langle f_n | \Psi \rangle$

 $|c_n|^2$ is the probability that a measurement of Q will yield the value q_n .

Interpretations of $|c_n|^2$

$$\Psi(x,0) = \sum_{n} c_n f_n(x)$$
$$|c_n|^2, \text{ where } c_n = \langle f_n | \Psi \rangle$$

 $|c_n|^2$ as the probability that the particle which is now in the state Ψ will be in the state f_n subsequent to a measurement of Q.

The process of measurement 'collapses' the wavefunction Ψ into one of its many 'potentia' state f_n into reality with a probability $|c_n|^2$.

Normalisation of Ψ

Since
$$\Psi(x,0) = \sum_{n} c_n f_n(x)$$

is normalised, e.g.,

$$\langle \Psi | \Psi \rangle = 1$$

It can be proven mathematically that

$$\sum_{n} |c_n|^2 = 1$$

Interpretation: the sum over of all possible outcome of a measurement got to be unity.

Proof of
$$\sum |c_n|^2 = 1$$

$$1 = \langle \Psi | \Psi \rangle = \left\langle \left(\sum_{n'} c_{n'} f_{n'} \right)^n \middle| \left(\sum_{n} c_n f_n \right) \right\rangle$$
$$= \sum_{n'} \sum_{n} c_{n'}^* c_n \langle f_{n'} | f_n \rangle$$
$$= \sum_{n'} \sum_{n} c_{n'}^* c_n \delta_{n'n}$$
$$= \sum_{n'} c_n^* c_n = \sum_{n'} |c_n|^2$$

Expectation value of Q

$$\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle$$

$$= \langle \left(\sum_{n'} c_{n'} f_{n'} \right) | \left(\hat{Q} \sum_{n} c_{n} f_{n} \right) \rangle$$

$$= \langle \hat{Q} f_{n}(x) = q_{n} f_{n}(x)$$

$$\langle Q \rangle = \sum_{n} q_{n} |c_{n}|^{2}$$

Prove the last step (it's easy)

Continuous c.f. discrete spectrum

Discrete spectrum

Discrete eigenvalues q_n labeled by discrete variable n

$$\hat{Q}f_n(x) = q_n f_n(x)$$

$$\Psi(x,0) = \sum_{n} c_n f_n(x)$$

$$|c_n|^2$$
, where $c_n = \langle f_n | \Psi \rangle$

Continuous spectrum

Continuous, real eigenvalue q(z) labeled by continuous variable z; e.g., z = x or = p

$$\hat{Q}f_z(x) = q(z)f_z(x)$$

$$\Psi(x,0) = \int c(z)f_z(x)dz$$

$$|c(z)|^2 dz \text{ where } c(z) = \langle f_z | \Psi \rangle$$

q(z) real, continuous eigenvalues associated with Q

 $f_z(x)$ Diracorthonomalised eigenfunctions associated with

Statistical interpretation of momentum measurement

$$\hat{p}f_p(x) = pf_p(x)$$

$$f_p(x) = (1/\sqrt{2\pi\hbar}) \exp(ipx/\hbar)$$

$$\hat{p} = -i\hbar d/dx$$

$$c(p) = \langle f_p | \Psi \rangle$$

$$= \int_{-\infty}^{\infty} f_p^*(x) \Psi(x, t) dx$$

Momentum space wavefunction

$$c(p) = \langle f_p | \Psi \rangle = \int_{-\infty}^{\infty} f_p^*(x) \Psi(x, t) dx$$

$$\Phi(p,t) \equiv \langle f_p | \Psi \rangle$$

 $|\Phi(p,t)|^2 dp$ eigenva

is the probability to obtain an eigenvalue *p* in the range d*p* in an momentum measurement.

 $\Phi(p,t)$ is in fact the Fourier transform conjugate of $\Psi(x,t)$

Fourier conjugate pair

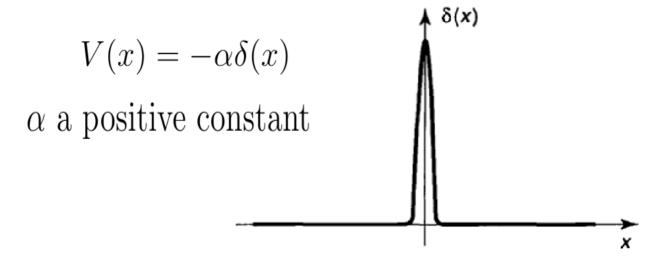
$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp(ipx/\hbar) \Phi(p,t) dp$$

"wave function in position space"

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp(-ipx/\hbar) \Psi(x,t) dx$$

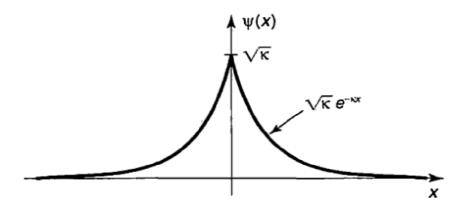
"wave function in momentum space"

Example: Calculate *p* for particle in Dirac delta potential



A particle of mass m is found in the delta function well. What is the probability that a measurement of its momentum would yield a value greater than $p_0 = m\alpha l \hbar$?

Calculate *p* for particle in Dirac delta potential



$$\Psi(x,t) = \frac{\sqrt{m\alpha}}{\hbar} \exp(-m\alpha|x|/\hbar^2) \exp(-iEt/\hbar)$$

$$E = -m\alpha^2/2\hbar^2$$

The momentum space wave function

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp(-ipx/\hbar) \Psi(x,t) dx$$

Calculate *p* for particle in Dirac delta potential

$$\Phi(p,t)$$

$$= \frac{\sqrt{m\alpha}}{\hbar} \frac{\exp(-iEt/\hbar)}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp(-ipx/\hbar) \exp(-m\alpha|x|/\hbar^2) dx$$

$$= \sqrt{\frac{2}{\pi}} \frac{p_0^{3/2} e^{-iEt/\hbar}}{p^2 + p_0^2}.$$
 Show this. Hint: use integral table, e.g., Spiegel

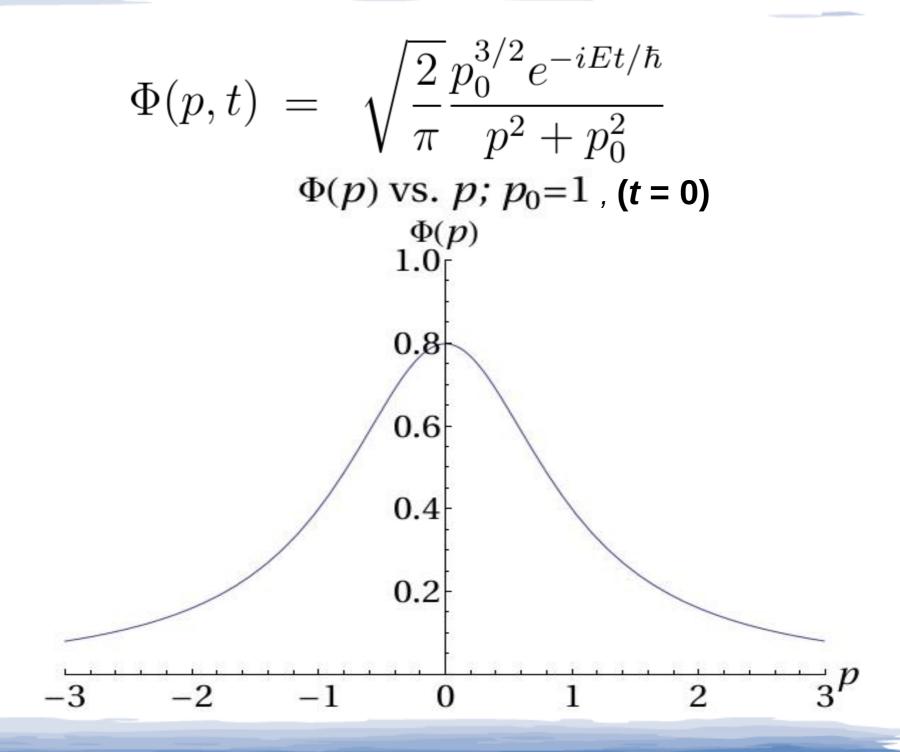
Note: m, lpha and \hbar are expressed in terms of $p_0=mlpha/\hbar$

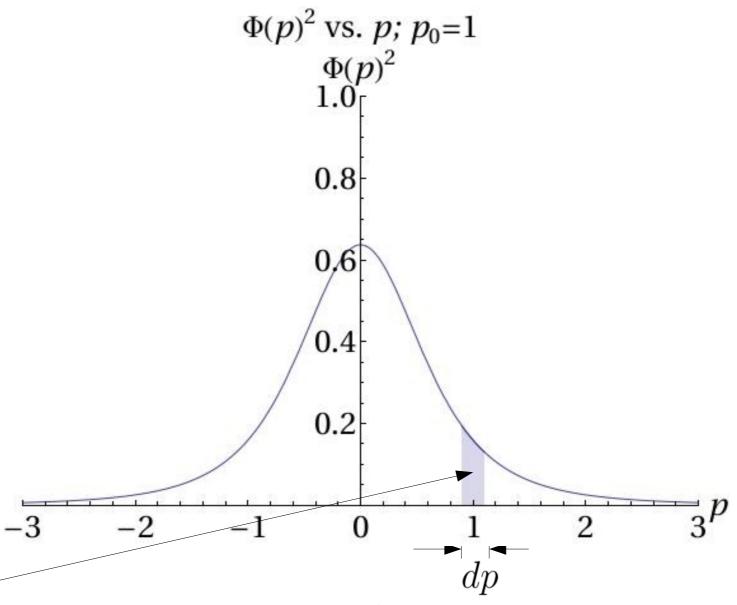
Calculate *p* for particle in Dirac delta potential

$$\Phi(p,t) = \sqrt{\frac{2}{\pi}} \frac{p_0^{3/2} e^{-iEt/\hbar}}{p^2 + p_0^2}$$

The probability to measure the momentum to lie between p and $p \pm dp$ is

$$Prob(p \pm dp) = |\Phi(p,t)|^2 dp$$
$$= \frac{2}{\pi} \frac{p_0^3}{(p^2 + p_0^2)^2} dp$$

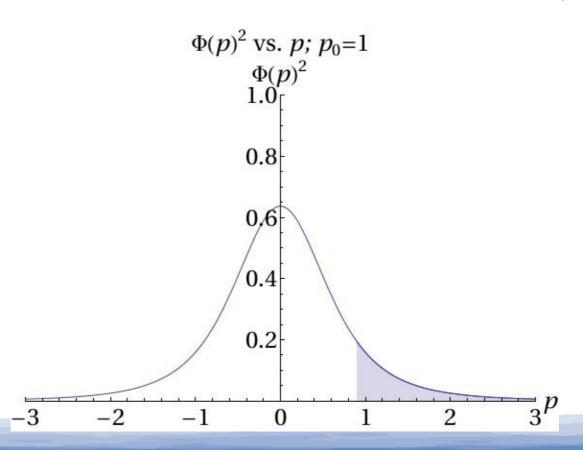




Shaded area showing probability to find particle with momentum lying in $p_0 \pm dp$

The probability to measure the momentum p to lie above p_0 is simply

$$\operatorname{Prob}(p > p_0) = \int_{p_0}^{\infty} |\Phi(p, t)|^2 dp = \frac{2}{\pi} \int_{p_0}^{\infty} \frac{p_0^3}{(p^2 + p_0^2)^2} dp$$
$$= \frac{2}{\pi} \left[\frac{pp_0}{p^2 + p_0^2} + \tan^{-1} \left(\frac{p}{p_0} \right) \right]_{p_0}^{\infty} = \frac{1}{4} - \frac{1}{2\pi}$$



Generalised uncertainty principle

Variances of two observables

Consider two observables A and B and their variances:

$$\begin{split} \sigma_A^2 &= \langle (\hat{A} - \langle A \rangle) \Psi | (\hat{A} - \langle A \rangle) \Psi \rangle = \langle f | f \rangle \\ \text{where } f &= (\hat{A} - \langle A \rangle) \Psi \\ \sigma_B^2 &= \langle (\hat{B} - \langle B \rangle) \Psi | (\hat{B} - \langle B \rangle) \Psi \rangle = \langle g | g \rangle \\ \text{where } g &= (\hat{B} - \langle B \rangle) \Psi \end{split}$$

Applying Schwarz inequality to the products of variances

Due to Schwarz inequality

$$\sigma_A^2 \sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \ge |\langle f|g\rangle|^2$$

Eq. (1)

Look at $|\langle f|g\rangle|^2$

Let $z \equiv \langle f|g\rangle$ (a complex number)

For any complex number z,

$$|z|^2 = (\operatorname{Im} z)^2 + (\operatorname{Re} z)^2 \ge (\operatorname{Im} z)^2 = \left[\frac{1}{2i}(z - z^*)\right]^2$$

In terms of f and g , Eq. (2) becomes

$$|\langle f|g\rangle|^2 \ge \left[\frac{1}{2i}(\langle f|g\rangle - \langle f|g\rangle^*)\right]^2 = \left[\frac{1}{2i}(\langle f|g\rangle - \langle g|f\rangle)\right]^2$$

Eq. (3)

$z - z^*$, in terms of commutator of A and B

Independently, one can show that

$$z = \langle f|g\rangle = \cdots \langle \hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle$$

$$z^* = \langle g|f\rangle = \cdots \langle \hat{B}\hat{A}\rangle - \langle B\rangle\langle A\rangle \quad \text{(Show these)}$$

$$z-z^*=\langle f|g\rangle-\langle g|f\rangle=\langle \hat{A}\hat{B}\rangle-\langle \hat{B}\hat{A}\rangle=\langle [\hat{A},\hat{B}]\rangle$$
 Eq. (4)

where the commutator of the operators A and B is defined as

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

Show the last step in Eq. (4)

Putting everything together

$$\sigma_A^2 \sigma_B^2 \ge |\langle f|g\rangle|^2$$

$$|\langle f|g\rangle|^2 \ge \left[\frac{1}{2i}(\langle f|g\rangle - \langle g|f\rangle)\right]^2$$
$$\langle f|g\rangle - \langle g|f\rangle = \langle \hat{A}\hat{B}\rangle - \langle \hat{B}\hat{A}\rangle = \langle [\hat{A}, \hat{B}]\rangle$$

$$\sigma_A^2 \sigma_B^2 \ge \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle\right)^2$$

This is the generalised uncertainty principle

It is a mathematical result

 Note that the generalised uncertainty relation is a consequence of the mathematical properties of Hermitian operators living in the Hilbert space and complex number.

Canonical commutator relation

$$[\hat{x}, \hat{p}] = i\hbar$$

This is an axiom (a principle that is generally assumed to be true) in QM.

Plug it into the generalised uncertainty relation gives

$$\sigma_x^2 \sigma_p^2 \ge \left(\frac{1}{2i}i\hbar\right)^2 = (\hbar/2)^2$$
$$\sigma_x \sigma_p \ge \hbar/2$$

Heisenberg's uncertainty principle is recovered!!!

Note on the derivation of HUP

$$\sigma_x \sigma_p \geq \hbar/2$$

- Heisenberg's uncertainty principle is recovered as a mathematical consequence of
 - (1) the canonical commutator relation axiom

$$[\hat{x}, \hat{p}] = i\hbar$$

(2) generalised uncertainty relation

$$\sigma_A^2 \sigma_B^2 \ge \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle\right)^2$$

Incompatible observables

 A pair of incompatible observables, say {A, B}, is one whose operators do not commute,

$$[A, B] \neq 0$$

Incompatible observables do not have shared eigenfunctions.

• i.e, if f(x) is an eigenfunction of operator A, it cannot be an eigenfunction of B, or vice versa.

Note on the symbol for operator and observable

The symbol for "operator" and "observable" is often used interchangeably

 For example, A can be referred to as "observable" or "operator".

 Which one it represents can be inferred from the context.

Proof by contradiction

Let A, B be two incompatible observables, hence,

$$[A, B] \neq 0$$

 We will prove that they don't share a common (simultaneous) eigenfunction by using "proof by contradiction":

Assume A, B share a common eigenfunction g.

$$Ag = ag, Bg = bg$$

where a, b eigenvalues corresponds to A and B.

$$[A, B] g = (AB - BA) g = (ab - ba)g = 0,$$

which is a contradiction to $[A, B] \neq 0$

Hence, g cannot be a common eigenfunction to A and B.

Example of incompatible observables

•*x* and *p*

$$[\hat{p}, \hat{x}] = -i\hbar \neq 0$$

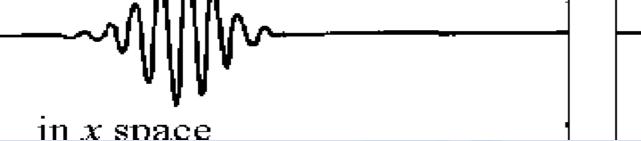
•There is no eigenfunction of position that is also an eigenfunction of momentum:

$$\hat{p}f(x) = pf(x), \hat{x}g(x) = xg(x) \Rightarrow f(x) \neq g(x)$$

Consecutive measurements of two incompatible observables

• For incompatible observables *A* and *B*, the results of the measurement of *A* will be rendered obsolete by the subsequent measurement of *B* (think of measuring momentum followed by measuring the position).





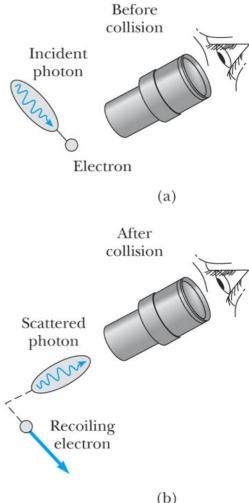
in k space

Heisenberg's Gedanken experiment

Illustrate very well the incompatibility of measuring x and p of a photon

x and p of a photon cannot be known simultaneously.

x and p are incompatible observables.



Compatible observables

If [A, B] = 0, then A, B are compatible (commuting) observables

They share a complete set of common (simultaneous) eigenfunctions.

Example of commuting observables: H, L^2 , and L_2

$$\mathcal{H}f(x) = Ef(x).$$

$$\hat{L}^2 f(x) = \ell(\ell+1)\hbar^2 f(x)$$

$$\hat{L}_z f(x) = \hbar m_\ell f(x)$$

Consecutive measurements of two compatible observables

If observables A and B are compatible, the result of the A measurement will not effect the result of the measurement of B subsequently (think of measuring energy followed by total angular momentum)

Analogy

Compatible observables are like friendship;

Incompatible observables are like romance.

Other uncertainty relations

Other than the famous Heisenberg uncertainty relation,

$$\sigma_x \sigma_p \geq \hbar/2$$

there exist many other very important results from the generalised uncertainty principle.

$$\sigma_A^2 \sigma_B^2 \ge \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle\right)^2$$

Uncertainty relation for Hamiltonian and position

Exercise: Show that $[H,x] = -\frac{i\hbar p}{m}$

Hence, show that $\sigma_H \sigma_x \geq \frac{\hbar |\langle p \rangle|}{2m}$

Hint: you need this

$$[AB, C] = A[B, C] + [A, C]B$$

and

$$[\hat{x},\hat{p}]=i\hbar$$

Uncertainty relation for Hamiltonian and momentum

Exercise: Show that $[H, p] = i\hbar \frac{d}{dx}V(x)$. Hence, show that $\sigma_H \sigma_p \geq \frac{\hbar}{2} \langle \frac{dV(x)}{dx} \rangle$

Hint: you need this

$$[f(x), p] = i\hbar \frac{df(x)}{dx}$$

and

$$[\hat{x},\hat{p}]=i\hbar$$

The Energy-Time Uncertainty Principle

$$\Delta E \Delta t \geq \hbar/2$$

The time variable, t

• Dynamical obserables are treated on very unequal footing in the QM (see the Schroedinger Equation)

 $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$

Time is not dynamical observable like others (E, p, x, etc.).

You don't measure "time" of a particle as you might its position or energy.

Time is an independent variable.

Dynamical observables are function of time.

Comparing $\Delta E \Delta t \geq \hbar/2$ against $\sigma_x \sigma_p \geq \hbar/2$

In non-relativistic QM,

$$\Delta E \Delta t \geq \hbar/2$$

cannot be derived from

$$\sigma_x \sigma_p \ge \hbar/2$$

 σ_q in the uncertainty relation is standard deviation of a collection of the measurement of observable Q

In contrast, Δt is not the standard deviation of a collection of the measurement of time. It is ...

 Δt is ...

$$\Delta E \Delta t \geq \hbar/2$$

The time it takes the system to change substantially

- How to quantify the time for a 'substantial change'
- That depends on how fast the system changes

Quantifying how fast a system is changing

 The rate of change of the expectation value of an observable

$$\frac{d}{dt}\langle Q\rangle$$

- It tells us how fast an the expectation value of an observable *Q* is changing in time
- This is the quantity we would monitor to quantify "how fast a system is changing"

Expanding $\frac{d}{dt}\langle Q \rangle$

$$\begin{split} \frac{d}{dt} \langle Q \rangle &= \frac{d}{dt} \langle \Psi | \hat{Q} \Psi \rangle \\ &= \langle \frac{\partial \Psi}{\partial t} | \hat{Q} \Psi \rangle + \langle \Psi | \frac{\partial \hat{Q}}{\partial t} \Psi \rangle + \langle \Psi | \hat{Q} \frac{\partial \Psi}{\partial t} \rangle \end{split}$$

$$\frac{\partial \Psi}{\partial t} = \frac{1}{i\hbar} \hat{H} \Psi$$
 — The TD Schroedinger equation

$$\frac{d}{dt}\langle Q\rangle = -\frac{1}{i\hbar}\langle \hat{H}\Psi|\hat{Q}\Psi\rangle + \frac{1}{i\hbar}\langle \Psi|\hat{Q}\hat{H}\Psi\rangle + \langle \frac{\partial Q}{\partial t}\rangle
= \frac{i}{\hbar}\langle [\hat{H},\hat{Q}]\rangle + \langle \frac{\partial Q}{\partial t}\rangle$$

Show this

$$-\frac{1}{i\hbar}\langle \hat{H}\Psi|\hat{Q}\Psi\rangle + \frac{1}{i\hbar}\langle \Psi|\hat{Q}\hat{H}\Psi\rangle = \frac{i}{\hbar}\langle [\hat{H},\hat{Q}]\rangle$$

Hint: The Hamiltonian *H* is hermitian

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}]\rangle$$

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}]\rangle + \langle \frac{\partial Q}{\partial t}\rangle$$

Typically, \hat{Q} does not depend on time explicitly,

$$\frac{\partial \hat{Q}}{\partial t} = 0$$

$$\Rightarrow \langle \frac{\partial \hat{Q}}{\partial t} \rangle = 0.$$

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}]\rangle$$

Interpretation of

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}]\rangle$$

The equation tells us how the expectation value of *Q* evolves in time

The evolution is dependent of commutator of the operator Q with the Hamiltonian.

Deriving Ehrenfest's theorem

Ehrenfest's theorem: expectation values obey classical laws

Examples:

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle$$

$$\frac{d}{dt}\langle p\rangle = -\langle \frac{dV(x)}{dx}\rangle$$

The above relations can be derived from

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}]\rangle$$

Show this

Observable Q is a conserved quantity if commute with H

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}]\rangle$$

- If [Q, H] = 0, then $\langle Q \rangle$ is constant in time.
- Q is a conserved quantity.

Deriving
$$\sigma_H \sigma_Q \geq \left(\frac{\hbar}{2}\right) \left|\frac{d\langle Q\rangle}{dt}\right|$$

Applying the generalised uncertainty principle to a generic operator Q and the Hamiltonian H

$$\sigma_A^2 \sigma_B^2 \ge \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle\right)^2$$

$$A \to H, B \to Q$$

$$\sigma_H^2 \sigma_Q^2 \ge \left(\frac{1}{2i} \langle [\hat{H}, \hat{Q}] \rangle \right)^2 = \left(\frac{1}{2i} \frac{\hbar}{i} \frac{d}{dt} \langle Q \rangle \right)^2 = \left(\frac{\hbar}{2}\right)^2 \left(\frac{d \langle Q \rangle}{dt}\right)^2$$

$$\sigma_H \sigma_Q \ge \left(\frac{\hbar}{2}\right) \left|\frac{d\langle Q\rangle}{dt}\right|$$

Interpreting
$$\sigma_H \sigma_Q \geq \left(\frac{\hbar}{2}\right) \left|\frac{d\langle Q\rangle}{dt}\right|$$

Rearrange:

Rearrange:
$$\sigma_{H} \cdot \frac{\sigma_{Q}}{\left|\frac{d\langle Q\rangle}{dt}\right|} \geq \frac{\hbar}{2}$$
Compare this with
$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Identify the following quantities

$$\Delta E \equiv \sigma_H$$
 $\Delta t \equiv \frac{\sigma_Q}{|d\langle Q\rangle/dt|}$

Interpretation of Δt

The change of expectation value of Q in time Δt is related via the definition

$$\Delta t \equiv \frac{\sigma_Q}{|d\langle Q\rangle/dt|} \longrightarrow \sigma_Q = \left|\frac{d\langle Q\rangle}{dt}\right| \Delta t$$

We are now ready to interpret Δt :

 Δt represents the the amount of time it takes the expectation value of Q to change by one standard deviation.

Δt varies from observable to observable

$$\sigma_Q = \left| \frac{d\langle Q \rangle}{dt} \right| \Delta t$$

 Δt varies from one observable to observable, because different Q has a different $\frac{d\langle Q \rangle}{dt}$

Fast changing observable has large uncertainty in energy

If any observable changes rapidly,

$$\left| \frac{d\langle Q \rangle}{dt} \right| >> 1$$

that means $\Delta t \ll 1$

as
$$\sigma_{\!\scriptscriptstyle Q}$$
 in $\sigma_{\!\scriptscriptstyle Q}=\left|\frac{d\langle Q\rangle}{dt}\right|\Delta t$ is fixed to 1 standard

deviation in the definition of Δt .

The "uncertainty" (ΔE) must be large according to $\Delta E \Delta t \geq \frac{h}{2}$

The specific meaning of Δt varies from case to case

• Δt as appeared in $\Delta t \Delta E \geq \hbar/2$ has a variety of specific meanings, depending on the context of the system being considered.

• The best way to understand the meaning of Δt is by looking at many different examples.

Example 1: Δt in the oscillation of a mixed state

A stationary state has definite energy, so $\Delta E = 0$, $\Delta t \rightarrow \infty$. But for a mixture of two stationary states, we could show that the product of ΔE and Δt obey the uncertainty bound.

Example 1 (cont. 1)

A linear combination of two stationary states

$$\Psi(x,t) = a\psi_1(x)e^{-iE_1t/\hbar} + b\psi_2(x)e^{-iE_2t/\hbar},$$
where $a, b, \psi(x), \psi(x)$ are real

$$|\Psi(x,t)|^2 = a^2 \psi_1(x)^2 + b^2 \psi_2(x)^2 + 2ab\psi_1(x)\psi_2(x)\cos\left(\frac{E_2 - E_1}{\hbar}t\right)$$

The period of oscillation is $\tau = 2\pi\hbar/(E_2 - E_1)$

Note:
$$\frac{(E_2 - E_1)}{\hbar} t = \frac{\Delta E}{\hbar} t \equiv \omega t \Rightarrow \Delta E = \hbar \omega; \omega = \frac{2\pi}{\tau}$$

Example 1 (cont. 2)

Taking $\Delta t = \tau$

$$\tau = 2\pi\hbar/(E_2 - E_1)$$

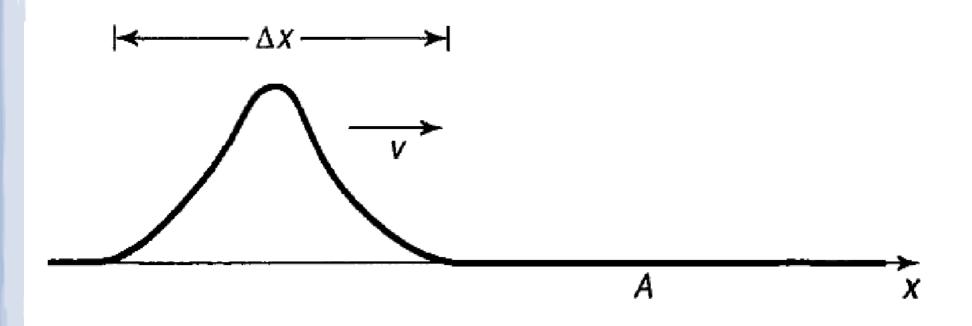
then implies

$$\Delta E \Delta t = 2\pi \hbar > \frac{\hbar}{2}$$

We have just shown that the energy-time uncertainty principle is respected in the system.

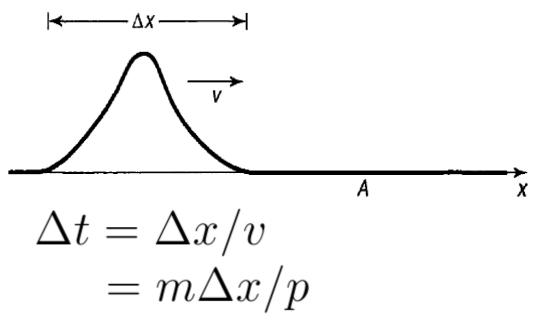
Example 2: Δt in the motion of a free-particle wave

How long does it take a free-particle wave packet to pass by a particular point?



A free particle wave packet approaches the point A (Example 3.6).

Example 2 (cont.)



But
$$E = p^2/2m$$
, so $\Delta E = p\Delta p/m$

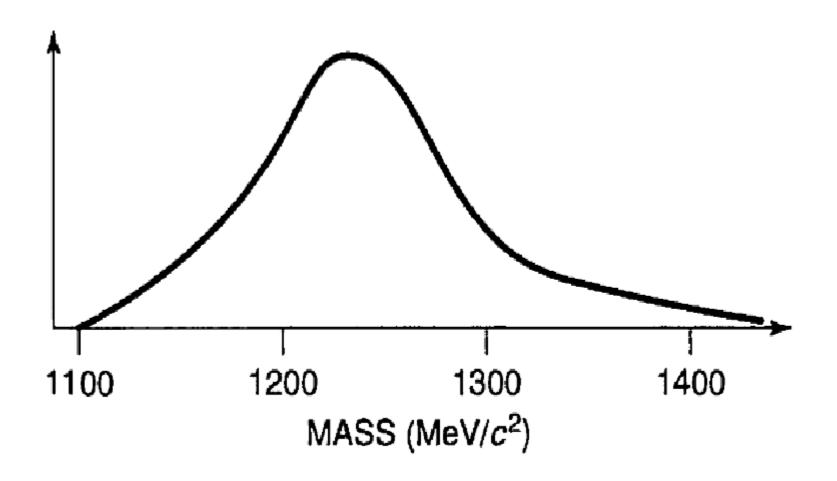
$$\Delta E \Delta t = \frac{p\Delta p}{m} \frac{m\Delta x}{p} = \Delta x \Delta p$$

$$\geq \hbar/2$$

We have just shown that the energy-time uncertainty principle is respected in the system.

Example 3: Δt in the decay of the Δ particle

The Δ particle last about 10^{-23} seconds, before spontaneously disintegrating. If you make a histogram of all measurements of its mass, you get a kind of bell-shaped curve centered at 1232 MeV/ c^2 , with a width of about 120 MeV/ c^2 . Why does the rest energy mc^2 sometimes come out higher that 1232, and sometimes lower? Is this experimental error?



Histogram of measurements of the Δ mass (Example 3.7).

Example 3 (cont. 1)

- The 'spread' of the rest energy (equivalent to the rest mass) of Δ particle, ΔE =120 MeV/ c^2 is consistent with the energy-time uncertainty relation.
- You can check that indeed

$$\Delta E \Delta t = \left(\frac{120}{2} \text{MeV}\right) (10^{-23} \text{sec})$$

$$= 6 \times 10^{-22} \text{MeV sec}$$

$$\geq \hbar/2 = 3 \times 10^{-22} \text{ MeV sec}$$

Example 3 (cont. 2)

- The rest mass of the Delta particle is not sharply defined (unlike many other stable particles, e.g, electron and proton).
- The 'spread' of the rest energy (rest mass) of the Δ particle is an inherent uncertainty that arises due to the time-energy uncertainty principle.
- The rest mass of the particle has a large 'spread' (uncertainty) of the order ~MeV/c² because of its short lifetime, 10⁻²³ sec (strong interactions).
- The shorted the lifetime of a particle the larger is the uncertainty of its rest mass.

Example 3 (cont. 3)

- How large the value of ΔE of a particle depends on the lifetime, $t=\Delta t$, which in turns depend on the fundamental interactions acting on the particles (strong forces, weak forces or electromagnetic forces).
- As long as the value of ΔE fulfills the condition that product of ΔE and Δt is less than $\hbar/2$, it will be allowed to happen, such as in the case of the Delta particle.

We have just shown that the energy-time uncertainty principle is respected in the system.

To sum up

- In the previous examples, Δt takes on a variety of specific meaning.
- In Example 1: it's a period oscillation.
- In Example 2, it's the time it takes a particle to pass a point
- In Example 3, it's the lifetime of an unstable particle.
- In these examples, Δt is the time it takes for the system to undergo "substantial" change.