0.1 Lecture IV

0.1.1 Particle in 1 D

We now look at a true Hilbert space, whose dimension is non-denumerable and infinite. A particle of mass m is constrained to move in one dimension, whose position coordinate is x. We denote the position operator $\hat{x}$ and define its eigenstates

$$\hat{x}|x>= x|x> \tag{1}$$

Note that x is no longer discrete since a measurement with device $\hat{x}$ can produce any value in the domain of real numbers. Thus the basis $|x>$ span an infinite vector space. If this basis is complete we can express a quantum state $|\Psi>$,

$$|\Psi>= \sum_x \Psi(x)|x> \tag{2}$$

in analogy with the expansion over a complete discrete basis

$$|\Psi>= \sum_n \Psi_n|n>, \tag{3}$$

where Ψ_n is the probability amplitude to find the system in state $|n>$. However the sum $\sum_x$ is undefined since x is non-denumerable. We substitute $\sum_x \rightarrow \int dx$ i.e. the sum becomes an integral. The probability to find the system in the region $x, x+dx$ is given by

$$dx|\Psi(x)|^2 \tag{4}$$

In analogy with the discrete case, $\Psi(x)$ is called the probability amplitude at point x, it is a function of a continuous variable x. For the discrete case, the amplitude is given by the relation $\Psi_n =< n|\Psi>$, so we require (assuming $|x>$ are orthogonal)

$$\Psi(x) =< x|\Psi> \tag{5}$$

Inserting this relation above we get

$$|\Psi>= \int dx \ < x|\Psi> |x> \tag{6}$$

Lets take the inner product of the above relation with ket $|x'>$

$$< x'|\Psi >= \int dx \ < x|\Psi >< x'|x >$$

$$\Psi(x') = \int dx \, \Psi(x) < x'|x > \tag{7}$$

We know that the Dirac delta function (see appendix in text) has the property

$$\int dx\delta(x-a)f(x) = f(a) \tag{8}$$

where $f(x)$ is any arbitrary function of x. Comparing this relation with the equation derived above we require

$$< x|x' >= \delta(x - x'). \tag{9}$$

In matrix representation theory we pointed out that a set of amplitudes $< n|\Psi >$, representing the probability to find the system in state $|n >$, can be written as a column matrix

$$|\Psi >\to \begin{pmatrix} < 1|\Psi > \\ < 2|\Psi > \\ . \\ . \\ . \\ < n|\Psi > \end{pmatrix}. \tag{10}$$

We can arrange the amplitudes $\Psi(x)$ in the same way,

$$|\Psi >\to \begin{pmatrix} < x|\Psi > \\ < x'|\Psi > \\ . \\ . \\ . \\ < x''|\Psi > \end{pmatrix}. \tag{11}$$

We require that $< \Psi|\Psi >= 1$. Using the completeness relation

$$\int dx \, |x >< x| = I \tag{12}$$

we obtain

$$< \Psi|\Psi >= \int dx \ < \Psi|x >< x|\Psi >= \int dx \, \Psi^*(x)\Psi(x) = 1 \tag{13}$$

0.1.2 Momentum in 1 D

We denote the momentum operator $\hat{p}$ so that

$$\hat{p}|p>= p|p> \tag{14}$$

$|p>$ also represent a complete basis,

$$< p|p'>= \delta(p-p') \tag{15}$$

and we can define an amplitude $\Psi(p)$ so that

$$|\Psi>= \int dp|p>< p|\Psi>= \int dp|p> \Psi(p) \tag{16}$$

The operator $\hat{x}$, $\hat{p}$ are incompatible since

$$[\hat{p}, \hat{x}] = -i\hbar I. \tag{17}$$

Let us find the matrix representation of operator $\hat{x}$, $< x'|\hat{x}|x >$. This is the analog of the matrix element $x_{mn} =< m|\hat{x}|n >$ for a discrete basis. We find

$$< x'|\hat{x}|x >=< x'|x > x = x\delta(x-x') \tag{18}$$

we notice that the matrix is "diagonal". How about $< p'|\hat{x}|p >$? We note

$$< x'|(\hat{x}\hat{p}-\hat{p}\hat{x})|x >= (x'-x) < x'|\hat{p}|x > \tag{19}$$

but $[\hat{p}, \hat{x}] = -i\hbar I$ and so

$$(x'-x) < x'|\hat{p}|x >= i\hbar < x'|I|x >= i\hbar\delta(x-x') \tag{20}$$

we need to "solve" the above equation for $< x'|\hat{p}|x >$ we make the "guess"

$$< x'|\hat{p}|x >= -i\hbar\frac{\partial}{\partial x'}\delta(x'-x) \tag{21}$$

We justify this guess by inserting this relation into the Eq. above and find,

$$-i\hbar(x'-x)\frac{\partial}{\partial x'}\delta(x'-x) = -i\hbar\frac{\partial}{\partial x'}\Big[(x'-x)\delta(x'-x)\Big] + i\hbar\delta(x-x') \tag{22}$$

the first term is a total derivative, and if we integrate it we obtain a term proportional to $(x-x')\delta(x-x') = 0$. Thus

$$\begin{gathered} < x'|\hat{x}|x >= x\delta(x'-x) \\ < x'|\hat{p}|x >= -i\hbar\frac{\partial}{\partial x'}\delta(x'-x) \end{gathered} \tag{23}$$

HW Find the representation of $\hat{x}$ and $\hat{p}$ in the momentum basis.

Uncertainty principle

We took note that position $\hat{x}$ and momentum $\hat{p}$ are incompatible operators. Given that the system is in state $|\Psi>$ and that independent measurements lead to expectation values

$$\begin{aligned} <x> &= <\Psi|\hat{x}|\Psi> \\ <p> &= <\Psi|\hat{p}|\Psi>, \end{aligned} \tag{24}$$

we now discuss a relationship between the variance $\Delta x^2 \equiv <\hat{x}^2> - <\hat{x}>^2$ and $\Delta p^2 \equiv <\hat{p}^2> - <\hat{p}>^2$ We define operators

$$\begin{aligned} \Delta\hat{x} &\equiv \hat{x} - <\hat{x}> \\ \Delta\hat{p} &\equiv \hat{p} - <\hat{p}> \end{aligned} \tag{25}$$

given state $|\Psi>$ we can define new states

$$\begin{aligned} &\Delta\hat{x}|\Psi> \\ &\Delta\hat{p}|\Psi> \end{aligned} \tag{26}$$

since these states must satisfy the Schwarz inequality we get

$$<\Delta\hat{x}^2><\Delta\hat{p}^2> \quad \geq \quad |<\Delta\hat{x}\Delta\hat{p}>|^2 \tag{27}$$

but

$$\Delta\hat{x}\,\Delta\hat{p} = 1/2[\Delta\hat{x}, \Delta\hat{p}] + 1/2\{\Delta\hat{x}, \Delta\hat{p}\}_+ \tag{28}$$

where $\{A, B\}_+ \equiv AB + BA$. Now $[\Delta\hat{x}, \Delta\hat{p}] = [\hat{x}, \hat{p}]$ and so

$$<\Delta\hat{x}\Delta\hat{p}> = 1/2 <[\hat{x}, \hat{p}]> + 1/2 <\{\Delta\hat{x}, \Delta\hat{p}\}_+> \tag{29}$$

The operator $[\hat{x}, \hat{p}]$ is antihermitian since $[\hat{x}, \hat{p}]^\dagger = -[\hat{x}, \hat{p}]$ and one can show that the expectation value for an antihermitian operator is always a pure imaginary number, whereas the the expectation value of the hermitian operator $\{\Delta\hat{x}, \Delta\hat{p}\}_+$ is always real. Thus

$$|<\Delta\hat{x}\Delta\hat{p}>|^2 = 1/4|<[\hat{x}, \hat{p}]>|^2 + 1/4|<\{\Delta\hat{x}, \Delta\hat{p}\}_+>|^2 \tag{30}$$

It follows that

$$<\Delta\hat{x}^2><\Delta\hat{p}^2> \quad \geq \quad 1/4|<[\hat{x}, \hat{p}]>|^2 \tag{31}$$

We note that $<\Delta\hat{x}^2> = <\Delta x^2>$, and $<\Delta\hat{p}^2> = <\Delta p^2>$ and so we obtain, using the the commutator $[\hat{p}, \hat{q}] = -i\hbar I$,

$$<\Delta x^2><\Delta p^2> \geq \hbar^2/4 \tag{32}$$

0.1.3 Schroedinger equation

We consider the time-evolution equation

$$i\hbar\frac{\partial|\Psi(t)>}{\partial t} = H|\Psi>$$
$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{33}$$

Take the inner product of this equation with ket $|x>$, then the left hand side becomes

$$ih < x|\frac{\partial|\Psi(t)>}{\partial t} = ih\frac{\partial < x|\Psi(t)>}{\partial t} = ih\frac{\partial\Psi(x,t)}{\partial t} \tag{34}$$

Consider the the r.h.s.

$$< x|\frac{\hat{p}^2}{2m} + V(\hat{x})|\Psi(t)> \tag{35}$$

First,

$$< x|V(\hat{x})|\Psi(t) >= V(x) < x|\Psi(t) >= V(x)\Psi(x,t) \tag{36}$$

(can you prove the above relation?). Also

$$< x|\hat{p}^2|\Psi(t) >= \int dx' \int dx'' \; < x|\hat{p}|x' >< x'|\hat{p}|x'' >< x''|\Psi(t)> \tag{37}$$

but using a previous result, the double integral can be re-written

$$\int dx' \int dx'' \, (-i\hbar)\frac{\partial}{\partial x}\delta(x-x')(-i\hbar)\frac{\partial}{\partial x'}\delta(x'-x'')\Psi(x'',t) \tag{38}$$

which, when integrated, gives

$$-\hbar^2\frac{\partial^2}{\partial x^2}\Psi(x,t) \tag{39}$$

Thus we find the Schroedinger Eqn.

$$ih\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) \tag{40}$$

Momentum-coordinate transformation functions

Lets express an eigenstate of momentum $|p>$ in terms of the coordinate basis $|x>$

$$|p>=\int dx|x><x|p> \tag{41}$$

$<x|p>$ is a probability amplitude. If the system is in state $|p>$, it gives the probability to find it at position x, when a measurement with device $\hat{x}$ is made. Consider the identity,

$$<x|\hat{p}|p>=p<x|p> \tag{42}$$

but this can be re-written

$$\int dx' \; <x|\hat{p}|x'><x'|p>=p<x|p> \tag{43}$$

or

$$\int dx' \, (-i\hbar)\frac{\partial}{\partial x}\delta(x-x') <x'|p>=-i\hbar\frac{\partial}{\partial x}<x|p> \tag{44}$$

Thus

$$-i\hbar\frac{\partial\Phi(x)}{\partial x}=p\Phi(x) \tag{45}$$

where we defined $\Phi(x) \equiv <x|p>$. We can consider this equation as a differential equation for the function $\Phi(x)$, whose solution is

$$<x|p>=C\exp(ip\,x/\hbar) \tag{46}$$

where C is a constant.

We can find the constant C by requiring,

$$<p|p'>=\delta(p-p') \tag{47}$$

but

$$\begin{aligned} <p|p'> &= \int dx \; <p|x><x|p'>=\int dx|C|^2\exp(-i(p-p')/\hbar\,x) \\ &= |C|^2 2\hbar\pi\delta(p-p') \end{aligned} \tag{48}$$

where we have used the representation for the delta function,

$$\int dx \, \exp(i(p-p')x) = 2\pi\delta(p-p') \tag{49}$$

Thus

$$\Phi(x) \equiv < x|p >= \frac{1}{\sqrt{2\hbar\pi}} \exp(ip\,x/\hbar). \tag{50}$$

Note that

$$\int dx |\Phi(x)|^2 = \infty \tag{51}$$

Functions that are non-normalizable are called improper functions, typically physical states are represented by normalizable functions, so that

$$\int dx |\Psi(x)|^2 = 1. \tag{52}$$

By the Fourier theorem we can always represent a physical normalized function $\Psi(x)$ in terms of improper functions, e.g.

$$\Psi(x,t) = \frac{1}{\sqrt{2\hbar\pi}} \int \Psi(p,t) \exp(ip\,x/\hbar) \tag{53}$$

A normalized probability amplitude $\Psi(x,t)$ is also called a wavepacket.