Operators with Continuous Spectra

We have encounter operators whose spectra involve a finite number of eigenvalues such as $\hat{A}$ which is an angular momentum operator, or if it were solvable $\hat{H}$ for a finite well.

We have encountered operators with a infinite number of discrete eigenvalues like $\hat{H}$ for the simple harmonic oscillator.

The final class of operators are operators with a continuous spectrum like $\hat{X}$ and $\hat{P}$.

To answer questions about observations involving x and p we apply the same logic we have been using.

(1) To possible outcomes of a measurement of x or p are the eigenvalues x', p' of the corresponding operator

$$\hat{X}\,|x'\rangle = x'\,|x'\rangle$$

$$\hat{P}\,|p'\rangle = p'\,|p'\rangle$$

where $|x'\rangle$, $|p'\rangle$ is the eigenvecter associated with x', p'.

$\Rightarrow x', p'$ real numbers because $\hat{X}, \hat{P}$ Hermitian.

(2) The eigenvecters of $\hat{X}, \hat{P}$ form a complete set, so any state vector can be written as a linear combination

$$|\psi\rangle = \sum_{x'} c_{x'}\,|x'\rangle = \sum_{p'} c_{p'}\,|p'\rangle$$

This notation is somewhat unnatural if x', p' is continuous. It makes more sense to use functional notation for $c_{x'}$, $c_{p'}$

$$\psi(x') \equiv c_{x'}$$

$$\Psi(p') \equiv c_{p'}$$

Since the set of eigenvectors is complete, there exists a closure relation

$$\sum_{x'} |x'\rangle\langle x'| = \hat{1}$$

or more naturally since x' continuous

$$\int_{-\infty}^{\infty} |x\rangle\langle x|\, dx = \hat{1}$$

$$\int_{-\infty}^{\infty} |p\rangle\langle p|\, dp = \hat{1}$$

I have dropped the primes since the integration variable is always a dummy variable.

With the change in notation, the expansion of the state vector becomes

$$|\psi\rangle = \int_{-\infty}^{\infty} \psi(x)\,|x\rangle\,dx$$

$$|\psi\rangle = \int_{-\infty}^{\infty} \overline{\Psi}(p)\,|p\rangle\,dp$$

4 Our vectors live in a vector space with an inner product, $\langle f|g\rangle$. ~~We can express~~

~~this inner product~~ for the expansion of

~~$|f\rangle$ and $|g\rangle$ in~~ the eigenvectors of $\hat{X}$ and $\hat{P}$.

~~Define $f(x) = \langle$~~

Two eigenvectors with different eigenvalues must be orthogonal

$$\langle x'|x''\rangle = \delta_{x'x''}$$

$$\langle p'|p''\rangle = \delta_{p'p''}$$

But that doesn't work either, the Kronecker delta becomes the Dirac Delta function when the index becomes continuous.

$$\langle x' | x'' \rangle = \delta(x' - x'')$$

$$\langle p' | p'' \rangle = \delta(p' - p'')$$

5 Fourier's Trick - Once we have orthogonality we can use Fourier's Trick to pick off the coefficients.

For the discrete case, if $\{|\phi_i\rangle\}$ is an orthonormal basis then

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle$$

$$c_i = \langle \phi_i | \psi \rangle$$

For the continuous case

$$|\psi\rangle = \int \psi(x) |x\rangle \, dx$$

$$\psi(x') = \langle x' | \psi \rangle$$

$$= \int \psi(x) \langle x' | x \rangle \, dx$$

$$= \int \psi(x) \delta(x'-x) \, dx$$

$$= \psi(x') \quad \checkmark$$

<u>Wave function</u>

Likewise,

$$\overline{\psi}(p') = \langle p' | \psi \rangle$$

Momentum Space Wave function

6 <u>Inner Products</u> - With the above, we can move our abstract definition of the inner product, $\langle f|g \rangle$, to function space.

$$f(x) \equiv \langle x | f \rangle$$

$$g(x) \equiv \langle x | g \rangle$$

$$\langle f|g \rangle = \langle f | \hat{1} | g \rangle = \int dx \langle f|x \rangle \langle x|g \rangle$$

closure

$$= \int dx \, f^*(x) \, g(x)$$

7 <u>Wave functions</u> - $\psi(x) = \langle x|\psi\rangle$ is the component representation of the state vector $|\psi\rangle$ with inner product $\int dx\, f^* g\, dx = \langle f|g\rangle$.

$\Rightarrow$ $\psi(x)$ is vector in Hilbert Space (L^2), the space of <u>square-integrable</u> functions.

$\Rightarrow$ Dfn Square-Integrable $\left|\int dx\, \psi^* \psi\right| < \infty$

$\Rightarrow \langle\psi|\psi\rangle < \infty$

	Discrete	Continuous
Ket	$\vert\phi_n\rangle$	$\vert x\rangle$
Components	$c_n = \langle\phi_n\vert\psi\rangle$ $\vert\psi\rangle = \sum c_n \vert\phi_n\rangle$	$\psi(x) = \langle x\vert\psi\rangle$ $\vert\psi\rangle = \int \psi(x)\vert x\rangle dx$
Orthogonality	$\langle\phi_n\vert\phi_{n'}\rangle = \delta_{nn'}$	$\langle x\vert x'\rangle = \delta(x-x')$
Closure	$\hat{1} = \sum_n \vert\phi_n\rangle\langle\phi_n\vert$	$\hat{1} = \int dx\, \vert x\rangle\langle x\vert$

8 **Observations and Probability** Given $|\psi\rangle$ what values of x or p can be observed with what probability.

If the spectrum were discrete

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle \qquad A|\phi_n\rangle = a_n|\phi_n\rangle$$

then

$$P(a_n) = c_n^* c_n = |\langle\phi_n|\psi\rangle|^2$$

but suppose we want the probability of a range of outcomes

$$P(a_i \in [b,c]) = \sum_{a_i \in [b,c]} c_i^* c_i$$

Moving to the continuous spectrum

$$P(x \in [b,c]) = \sum_{x \in [b,c]} c_x^* c_x = \int_b^c \langle x|\psi\rangle^* \langle x|\psi\rangle \, dx$$

$$= \int_b^c |\langle x|\psi\rangle|^2 dx$$

Recalling continuous probability functions, the probability density for x is

$$\rho(x) = |\langle x | \psi \rangle|^2$$

$$P(x \in [b, c]) = \int_b^c \rho(x)\, dx$$

9 Eigenfunctions of $\hat{X}$, $\hat{P}$, $f_{x'}(x)$, $f_{p'}(x)$

$$f_{x'}(x) = \langle x | x' \rangle$$

eigenfunction of $\hat{X}$ with eigenvalue x'

$$f_{p'}(x) = \langle x | p' \rangle$$

eigenfunction of $\hat{P}$ with eigenvalue p'

From the postulates, the momentum operator in the position basis is

$$\hat{P} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

Eigenvalue equation

$$\hat{P} f_{p'}(x) = p' f_{p'}(x)$$

$$\frac{\hbar}{i} \frac{\partial}{\partial x} f_{p'}(x) = p' f_{p'}(x)$$

<u>Solution</u>

$$f_{p'}(x) = A e^{ip'x/\hbar}$$

<u>Normalize</u>

$$1 = \int_{-\infty}^{\infty} f_{p'}^* f_{p'} \, dx = AA^* \int dx = \infty$$

<u>Traditional Normalization</u>

$$f_{p'}(x) = \langle x | p' \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip'x/\hbar}$$

But what about, $f_{x'}(x) = \langle x | x' \rangle$

but we already know that by orthogonality

$$f_{x'}(x) = \delta(x - x')$$

(10) Connecting momentum and position space,

$$\overline{\Psi}(p) \equiv \langle p | \psi \rangle = \langle p | \hat{1} | \psi \rangle$$

$$= \int dx \, \langle p | x \rangle \langle x | \psi \rangle \quad \text{closure}$$

$$\langle p | x \rangle = \langle x | p \rangle^* = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}$$

$$\overline{\Psi}(p) = \int dx \, \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \psi(x)$$

or reversing the above

$$\psi(x) = \langle x | \psi \rangle = \langle x | \hat{1} | \psi \rangle$$

$$= \int dp \, \langle x | p \rangle \langle p | \psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dp \, e^{\frac{ipx}{\hbar}} \overline{\Psi}(p)$$

11 Briefly look at the delta function

$$\delta(x-x') = \langle x|x'\rangle = \int dp \langle x|p\rangle\langle p|x'\rangle$$

$$= \frac{1}{2\pi\hbar}\int dp\, e^{ipx/\hbar}\, e^{-ipx'/\hbar}$$

$$= \frac{1}{2\pi\hbar}\int dp\, e^{i(p-p')x/\hbar}$$

12 Representing Operators in Continuous Basis

In a discrete basis, an operator $\hat{A}$ was represented by a matrix. The equation

$$|b\rangle = \hat{T}|c\rangle$$

become

$$\begin{pmatrix} \langle a_1|b\rangle \\ \langle a_2|c\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} \langle a_1|\hat{T}|a_1\rangle & \langle a_1|\hat{T}|a_2\rangle & \cdots \\ \langle a_2|\hat{T}|a_1\rangle & \ddots & \\ \vdots & & \ddots \end{pmatrix} \begin{pmatrix} \langle a_1|c\rangle \\ \langle a_2|c\rangle \\ \vdots \end{pmatrix}$$

in the $\{|a_i\rangle\}$ basis.

Mothemotically

$$b_i \equiv \langle a_i | b_i \rangle = \langle a_i | \hat{T} | c \rangle$$

$$= \sum_j \langle a_i | \hat{T} | a_j \rangle \langle a_j | c \rangle$$

$$= \sum T_{ij} \, c_j$$

Consider the continuous vector equation

$$| g \rangle = \hat{X} | f \rangle$$

Take the ~~~~ components

$$g(x) = \langle x | g \rangle = \langle x | \hat{X} | f \rangle$$

what is $\langle x | \hat{X} | f \rangle$?

① $\langle x | (\hat{X} | f \rangle)$ which is no help

② $(\langle x | \hat{X}) | f \rangle = (\hat{X}^{+} | x \rangle)^{+}$

$$= (\hat{X} | x \rangle)^{+} = (x | x \rangle)^{+} = \langle x | x$$

Using the fact that $\hat{X}$ is Hermitian

$$g(x) = \langle x | \hat{X} | f \rangle = x \langle x | f \rangle = x f(x)$$

$\Rightarrow$ In the position basis, the effect of $\hat{X}$ on a wavefunction is to multiply the function by x.

<u>Now, what about $\hat{P}|f\rangle = |g\rangle$?</u>

$$g(x) = \langle x | \psi \rangle = \langle x | \hat{P} | f \rangle$$

but we don't know what $\hat{P}$ does to either $|x\rangle$ or $|f\rangle$ $\Rightarrow$ Use closure

$$g(x) = \langle x | \hat{1} \hat{P} | f \rangle = \int dp \langle x | p \rangle \langle p | \hat{P} | f \rangle$$

$$= \int dp \, p \langle x | p \rangle \langle p | f \rangle$$

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

$$g(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\left[\frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{ipx/\hbar}\,\bar{f}(p)\right]$$

$$= \frac{\hbar}{i}\frac{\partial}{\partial x} f(x)$$

$\Rightarrow$ The effect of $\hat{P}$ in the position basis is to operate with $\frac{\hbar}{i}\frac{\partial}{\partial x}$

There is nothing special about the position basis, sometimes other bases are more convienient.

<u>What is the effect of $\hat{P}$ in the momentum basis?</u>

$$\hat{P}|f\rangle = |g\rangle$$

$$\bar{g}(p) \equiv \langle p|g\rangle = \langle p|\hat{P}|f\rangle = p\langle p|f\rangle$$

$$= p\,\bar{f}(p)$$

$\Rightarrow$ The effect of $\hat{P}$ in the momentum basis is to multiply by p.

and $\hat{X}|f\rangle = |g\rangle$

$$\langle p|\hat{X}|f\rangle = \langle p|g\rangle = \bar{g}(p)$$

$$= \int dx \langle p|x\rangle\langle x|\hat{X}|f\rangle$$

$$= \int dx \langle p|x\rangle\, x \,\langle x|f\rangle$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int dx\, x\, e^{-ipx/\hbar} f(x)$$

$$= -\frac{\hbar}{i}\frac{\partial}{\partial p}\left[\frac{1}{\sqrt{2\pi\hbar}}\int dx\, e^{-ipx/\hbar} f(x)\right]$$

$$= -\frac{\hbar}{i}\frac{\partial}{\partial p}\bar{f}(p)$$

$\Longrightarrow$ The effect of $\hat{X}$ in the momentum basis is to operate with $\hat{X} = -\frac{\hbar}{i}\frac{\partial}{\partial p}$

13 Finally, the Schrodinger Eqn

By the same methods,

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

becomes

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

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t)$$

or if one likes

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

$$i\hbar \frac{\partial}{\partial t} \bar{\psi}(p,t) = \left[\frac{p^2}{2m} + V\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}\right) \right] \bar{\psi}(p,t)$$

A number not an operator

Let's solve the momentum SE for the free particle, $V(x) = 0$

$$i\hbar \frac{\partial}{\partial t} \Psi = \frac{p^2}{2m} \Psi(p,t)$$

$$\Psi(p,t) = A\, e^{\frac{p^2}{2m i\hbar} t}$$

$$= A\, e^{-iEt/\hbar}$$

if $E = \frac{p^2}{2m}$