Proof: Let $\mathbf{A} (\omega) \mathbf{r} = \omega_1 \mathbf{r}$

\[ \mathbf{r} = \sum_{n=1}^{\infty} \omega_n \mathbf{r}_n \]

Now consider the operator $\mathbf{U}$ which looks as follows:

\[ \mathbf{U} = \begin{pmatrix} \omega_{11} & \cdots & \omega_{1n} \\ \vdots & \ddots & \vdots \\ \omega_{n1} & \cdots & \omega_{nn} \end{pmatrix} \]

[Comment: $\mathbf{U}$ is a unitary matrix since $\mathbf{U}^\dagger \mathbf{U} = \mathbf{I}$]

First component of eigenvector of $\omega_1$.

$n$th component of normalized eigenvector of $\omega_1$.

1st component of eigenvector of $\omega_1$.

So columns are eigenvectors.

Then $\mathbf{S} (\omega) \mathbf{U} = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} \mathbf{U}$

\[ \begin{pmatrix} \omega_1 & \omega_2 & \cdots & \omega_n \\ \omega_1 & \omega_2 & \cdots & \omega_n \\ \vdots & \vdots & \ddots & \vdots \\ \omega_1 & \omega_2 & \cdots & \omega_n \end{pmatrix} \begin{pmatrix} \omega_{11} & \cdots & \omega_{1n} \\ \vdots & \ddots & \vdots \\ \omega_{n1} & \cdots & \omega_{nn} \end{pmatrix} \]
Then we can write

\[ U^* S U = \begin{pmatrix} w_1^* & \cdots & w_m^* \\ w_1 & \cdots & w_m \\ \vdots & \ddots & \vdots \\ w_1 & \cdots & w_m \end{pmatrix} \]

\[ = \begin{pmatrix} w_1 & 0 & \cdots & 0 \\ 0 & \ddots & \vdots & \vdots \\ \vdots & \ddots & w_n \\ 0 & \cdots & 0 & w_n \end{pmatrix} \]

since

\[ \sum_{k=1}^{n} w_k w_k^* = \delta_{ij} \text{ orthonormality} \]

Simultaneously

This procedure is called diagonalizing a Hermitean operator.
Thus: \( U^+ \Omega U \) is diagonal:

Theorem: If \( [\Omega, \psi] = 0 \) and \( \Omega \) and \( \Lambda \) are Hermitian, then there exists at least one basis of common eigenvectors which diagonalizes both. [They are "simultaneously diagonalizable"]

(for non-degenerate eigenvalues)

Proof: Suppose \( \Omega |w_i\rangle = \omega_i |w_i\rangle \)

Then \( \Lambda \Omega |w_i\rangle = \omega_i \Lambda |w_i\rangle \)

\[ = \Lambda \omega_i |w_i\rangle \]

Thus \( \Omega (\Lambda |w_i\rangle) = \omega_i (\Lambda |w_i\rangle) \)

Hence \( \Lambda |w_i\rangle \) is also an eigenvector of \( \Omega \)

with eigenvalue \( \omega_i \).

But \( |w_i\rangle \) was assumed unique to within a scale factor.

Therefore \( \Lambda |w_i\rangle \) is just a multiple of \( |w_i\rangle \)

i.e. \( \Lambda |w_i\rangle = \lambda_i |w_i\rangle \)

\( |w_i\rangle \) also an eigenvector of \( \Lambda \) with eigenvalue \( \lambda_i \).
Hence the basis \( \{ w_i \} \) diagonalizes both operators.

I.e., \( U^* \Sigma U = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_n \end{pmatrix} \)

and also \( U^* \Lambda U = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_n \end{pmatrix} \)

where \( U \) is the same in both cases.

How to treat degeneracies? I will just state that we can still use simultaneously diagonalize \( \Sigma \) and \( \Lambda \) with the same unitary matrix \( U \).

Functions of operators:

Let we consider only functions which can be represented as a power series (i.e. a Taylor series).

I.e., \( f(x) = \sum_{n=0}^{\infty} a_n x^n \)

Then \( f(U) = \sum_{n=0}^{\infty} a_n U^n \)
\[ e^{ax} = \sum_{n=0}^{\infty} \frac{(ax)^n}{n!} = \sum_{n=0}^{\infty} \frac{a^n x^n}{n!} \]

Then \( e^{\exp(a\Omega)} = \sum_{n=0}^{\infty} \frac{a^n \Omega^n}{n!} \)

Example: Let us consider only Hermitian operators \( \Omega \). Then in the basis in which \( \Omega \) is diagonal, we have

\[ \Omega = \begin{pmatrix} \omega_1 & & \\ & \ddots & \\ & & \omega_n \end{pmatrix} \]

with all the \( \omega_i \)'s real.

Then

\[ e^{\Omega} = \sum_{k=0}^{\infty} \frac{\Omega^k}{k!} \]

Now \( \Omega^2 = \)

because

\[ [\Omega, \Omega^2] = 0 \]

so

\[ \sum_{k=0}^{\infty} \frac{\Omega^k}{k!} = \begin{pmatrix} e^{\omega_1} & & \\ & \ddots & \\ & & e^{\omega_n} \end{pmatrix} \]
Exercise
Do exercises (1.9.2) and (1.9.3)

Derivatives of operators with respect to parameters

Suppose \( \Theta(\lambda) \) is an operator which depends on some parameter \( \lambda \).
Then the operator \( d\Theta/d\lambda \) is defined by
\[
\frac{d\Theta(\lambda)}{d\lambda} = \lim_{\Delta \lambda \to 0} \frac{\Theta(\lambda + \Delta \lambda) - \Theta(\lambda)}{\Delta \lambda}
\]

E.g. What is \( dA/d\lambda \) where
\[
A = \begin{pmatrix}
\lambda & 2\lambda + 3 \\
-\lambda^5 & \frac{1}{\lambda^2}
\end{pmatrix}
\]

Answer: \( \left( \frac{dA}{d\lambda} \right)_{ln} = \frac{dA_{mn}}{d\lambda} \)

So here \( dA = \begin{pmatrix}
1 & 2 \\
-5\lambda^4 & -\frac{2}{\lambda^3}
\end{pmatrix} \)

How about \( d\Theta/d\lambda \) where \( \Theta = e^{\lambda A} \)
Easiest to get via a power series:

\[
\frac{d}{d\lambda} \left( e^{\lambda \Omega} \right) = \frac{d}{d\lambda} \sum_{n=0}^{\infty} \frac{\lambda^n \Omega^n}{n!} = \sum_{n=0}^{\infty} \frac{n \lambda^{n-1} \Omega^n}{n!} = \sum_{n=0}^{\infty} \frac{\lambda^{n-1} \Omega^n}{(n-1)!} = \sum_{n=1}^{\infty} \frac{\lambda^{n-1} \Omega^n}{(n-1)!} = \sum_{n=0}^{\infty} \frac{\lambda^{n} \Omega^n}{n!} = e^{\lambda \Omega}.
\]

where we use:

\[
\frac{n}{n!} = \frac{1}{(n-1)!} = \frac{1}{(n-1)!}
\]

(because \( \frac{0^0}{0!} = 0 \)).

Change variables:

\[
\sum_{n=1}^{\infty} \frac{\lambda^{n-1} \Omega^n}{(n-1)!} = \sum_{m=0}^{\infty} \frac{\lambda^{m} \Omega^{m+1}}{m!}
\]

since where \( m = n-1 \)

\[
= \sum_{m=0}^{\infty} \frac{\lambda^{m} \Omega^{m+1}}{m!} = \sum_{m=0}^{\infty} \frac{\lambda^{m} \Omega^{m}}{m!} \Omega = \Omega e^{\lambda \Omega} = e^{\lambda \Omega} \Omega
\]

So the rule is:

\[
\text{If } f(\Omega) \text{ just take the derivative ignoring the fact that } f \text{ the function involves operators, not scalars.}
\]

Functions of more than one operator:

\[
\text{In this case, cannot generally}
\]
treat the functions as if they were just functions of scalars - i.e., they may not commute.

E.g. \( e^{\alpha \Omega} e^{\beta \Omega} = e^{(\alpha + \beta)\Omega} \) scalars

But \( e^{\alpha \Omega} e^{\beta \Theta} \neq e^{\alpha \Omega + \beta \Theta} \) in general

Partial proof: Consider second order term of second expression (i.e. terms of second order in \( \Omega \times \Theta \)) with \( x + y = 2 \)

Then we have:

\[
\left( \frac{\alpha \Omega}{2} \right)^2 + \alpha \beta \Omega \Theta + \left( \frac{\beta \Theta}{2} \right)^2 \quad \text{on the left}
\]

\[
\left( \frac{\alpha \Omega + \beta \Theta}{2} \right)^2 = \left( \frac{\alpha \Omega}{2} \right)^2 + \frac{\alpha \beta (\Omega \Theta + \Theta \Omega)}{2} + \left( \frac{\beta \Theta}{2} \right)^2 \quad \text{on the right}
\]

These are unequal unless \( [\Theta, \Omega] = 0 \).

Also \( e^{\alpha \Omega} e^{\beta \Theta} \neq e^{\beta \Theta} e^{\alpha \Omega} \) unless \( [\Omega, \Theta] \neq 0 \).
Generalization to infinite dimensions

Sounds unnecessary but is very important.

E.g., consider the set of all functions $f(x)$ in $a \leq x \leq b$

Well, do these functions form a vector space?

You can add two functions and get another.

Can multiply by a scalar and get another function.

But now consider how to find an orthonormal basis $f(x)$

Divide the interval $[a, b]$, $a \leq x \leq b$, into $n$ equal pieces. Represent the function $f(x)$ approximately by $f(x_i) \approx f(x)$, $i = 1, 2, \ldots, n$

where the $x_i$'s are equally spaced on the centers of the intervals.

E.g., $n = 6$

$\begin{align*}
\text{at } & x_1, x_2, x_3, x_4, x_5, x_6 \\
\text{at } & x_1, x_2, x_3, x_4, x_5, x_6
\end{align*}$
Then the function \( f(x) \) is represented by the \( n \)-dimensional ket

\[
| f_{\alpha n} \rangle \rightarrow \begin{pmatrix} f_{\alpha 1}(x_1) \\ f_{\alpha 2}(x_2) \\ \vdots \\ f_{\alpha n}(x_n) \end{pmatrix}
\]

for meaning approximate representation of \( f(x) \) by \( n \)-dimensional vector.

Basis vectors are

\[
| x_i \rangle \rightarrow \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \end{pmatrix}
\]

in the \( i \)-th place.

Or

\[
\text{function which = 1 at } x = x_i \\
= 0 \text{ elsewhere}
\]

With this definition,

\[
\langle x_i | x_j \rangle = \begin{pmatrix} 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix}
= \delta_{ij} \text{ (orthonormality)}
\]

and

\[
\sum_{i=1}^{n} | x_i \rangle \langle x_i | = I \text{ (completeness)}
\]

and

\[
| f \rangle = \sum_{i=1}^{n} f(x_i) | x_i \rangle
\]
Two functions \( f(x) \) and \( g(x) \) are called orthogonal if
\[
\langle f | g \rangle = \sum_{i=1}^{m} f(x_i) g(x_i) = 0
\]

Inner product
\[
\langle f | g \rangle = \sum_{i=1}^{m} f(x_i) g(x_i)
\]

(if we are dealing with real functions)

Now, let \( n \to \infty \). For large \( n \), we define
\[
\langle f | g \rangle = \sum_{i=1}^{m} \int_{a}^{b} f_{n}(x_i) g_{n}(x_i) \Delta x
\]
where \( \Delta = \frac{1}{n} \) with \( n \) the number of steps
\[
L = b - a \quad \text{the interval}
\]

In the limit \( n \to \infty \), we get
\[
\langle f | g \rangle = \int_{a}^{b} f(x) g(x) \, dx
\]
\[
\langle f | f \rangle = \int_{a}^{b} f^2(x) \, dx
\]

If we want to treat complex functions, we may define
\[
\langle f | g \rangle = \int_{a}^{b} f^*(x) g(x) \, dx
\]
How to define basis functions? Vectors?

We want $|x\rangle$ to be nonzero at pt. $x$ and zero elsewhere.

We also want $\langle x| x' \rangle = 0 \quad x' \neq x$

But what about $\langle x| x \rangle$?

Is $\langle x| x \rangle = 1$? No.

Why not? Well, we want

$$\int_0^L |x\rangle \langle x| \, dx' = 1$$

Now, left-multiply by $|x\rangle$ and right-multiply by $|f\rangle$.

Then we get

$$\langle x| \int_0^L |x'\rangle \langle x'| f \rangle \, dx' = \langle x| 1|f\rangle$$

$$= \langle x| f \rangle$$

But $\langle x| f \rangle = f(x)$ because the bra $\langle x|$ just projects out the corresponding part of the vector $|f(x)\rangle$.

Thus, we have

$$\int_0^L \langle x| x' \rangle f(x') \, dx' = f(x)$$
Now \(<x|\hat{x}^2|x>\) vanishes unless \(<x|\hat{x}|x> = x\) or very close to it

So we can take \(x\) replace \(f(x')\) in the integral by \(f(x)\). Thus we have

\[
\int_0^L \langle x|\hat{x}'|x> \, dx' \, f(x) = f(x) \quad \text{for any } f(x)
\]

In fact, integrand can be taken

\[
\int_0^L \langle x|\hat{x}'|x> \, dx' = 1
\]

(iif \(0 < x < L\))

Also \(<x|\hat{x}|x> = 0 \quad x \neq x'\)

This means, \(<x|\hat{x}|x> = \delta(x-x') = \text{Dirac delta function}\)

Dirac delta function satisfies:

\[
\delta(x-x') = 0 \quad x \neq x'
\]

\[
\int_{x_1}^{x_2} \delta(x-x') \, dx' = 1 \quad \text{if } x_1 < x < x_2
\]

\[
\int_{x_1}^{x_2} \delta(x-x') \, dx' = \infty \quad \text{at } x = x'
\]
Can think of \( \delta(x-x') = \lim_{\Delta \to 0} \frac{1}{\sqrt{\pi \Delta^2}} \exp \left( - \frac{(x-x')^2}{\Delta^2} \right) \) as a Gaussian of ever narrower width.

Thus we have our desired generalization.

Comments. \( \delta(x-x') \) is even, ie.

\[ \delta(x-x') = \delta(x'-x) \]

Proof: \( \delta(x-x') = \langle x | x' \rangle = \langle x' | x \rangle^* \)

\[ = \delta(x'-x)^* = \delta(x-x) \]

since the delta function is real.

Derivative of a delta function:

\[ \delta'(x-x') = \frac{d}{dx} \delta(x-x') = -\frac{d}{dx} \delta(x-x') \]

Consider:

\[ \int_a^b \delta'(x-x') f(x') dx' \]

where \( a < x' < b \)

\[ = \int_a^b \left[ \delta(x-x') f(x') \right] dx' - \int_{-a}^{a} \delta(x-x') f(x') dx' \]

\[ = \left[ \frac{f(x)}{\delta(x)} \right]_{-a}^{a} \]

\[ = \frac{f(a) - f(-a)}{\delta(x)} \]

\[ = \frac{f'(x)}{\delta(x)} \]
Operators in infinite dimensions.

\[ \Omega |\tilde{f}\rangle = |\tilde{f}\rangle \quad \text{\textit{\tilde{f}(x) = second function}} \]

E.g. \( D = \text{derivative operator} \)

\[ D|f\rangle = \int \frac{df}{dx} \langle x|f\rangle \]

or \( \langle x|D|f\rangle = \langle x| \frac{df}{dx} \rangle = \frac{df}{dx} \)

How so, what is \( \langle x|D|x\rangle \)?

Well \( \langle x|D|f\rangle = \int \langle x|D|x\rangle \langle x'|f\rangle dx' \) by completeness

\[ = \frac{df}{dx}(x) \]

\[ = \int \langle x|D|x\rangle f(x') dx' \]

which shows that \( \langle x|D|x\rangle = \delta(x-x') \frac{df(x)}{dx} \equiv D_{xx'} \)

Proof: \( \int \delta(x-x') \frac{df(x')}{dx'} dx' = \frac{df(x)}{dx} \equiv D_{xx'} \)

Alternate way of writing \( \langle x|D|x\rangle \):

\[ \int \langle x|^D|x\rangle \langle x'|f\rangle dx' = \int \delta(x-x') \frac{df(x')}{dx'} dx' \int \]
\[ \begin{align*}
&= - \int_a^b \frac{d}{dx} \delta(x-x') f(x') \, dx' \\
&= + \int_a^b \frac{d}{dx} \delta(x-x') f(x') \, dx' \\
&= \Rightarrow \langle x | D | x' \rangle = \frac{d}{dx} \delta(x-x') = \delta'(x-x')
\end{align*} \]

Is \( D \) Hermitian? No.

However, \( K = -iD \) is Hermitian.

**Proof:**

\[ D_{xx'} = \frac{d}{dx} \delta(x-x') \]

\[ D^*_{xx'} = D_{x'x} = \frac{d}{dx'} \delta(x'-x) = \frac{d}{dx'} \delta(x-x') = -\frac{d}{dx} \delta(x-x') \]

\[ = -D_{x'x} \]  

Since \( \delta(x-x') \) is an even function.

\[ \Rightarrow \quad \delta'(x-x') \]

But \( \delta'(x-x') = \text{undefined} \]

\[ = +iD_{x'x} = -iD_{x'x} = K_{xx'} \quad \text{so} \]

\[ K = \text{hermitian} \]

(Actually, not quite true always: have to worry about boundary conditions — see Shankar)
Eigenfunctions of $K$: 

$$<x|K|x> = k <x|x>$$

$$<x|K|x> = k <x|x> = k f_k(x)$$

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

$$= \int -i \frac{d}{dx} \delta(x-x') f_k(x') dx'$$

$$= \int \delta(x-x') \frac{d}{dx} f_k(x') dx'$$

$$= -i \int \delta(x-x') \frac{d}{dx} f_k(x') dx'$$

$$= -i \frac{d}{dx} f_k(x) = k f_k(x)$$

Solution: 

$$\frac{df_k(x)}{dx} = ikr$$

$$f_k(x) = Ae^{ikr}$$

$$f_k(x) = k <x|x>$$
Note: any real $k$ satisfies this condition, i.e. any real constant $k$ is an eigenvalue of $K$.

$A$ is a "normalization constant" — but if $x$ is an infinite interval, we cannot normalize $|k\rangle$.

Conventional choice for $A$: take $A = \frac{1}{\sqrt{2\pi}}$

With this choice,

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

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

Side mathematical comment: Why is

$$I = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} \, dx = \delta(k)?$$

Proof: Let $e^{-ikx} = \lim_{x' \to 0} e^{-ikx'}$

$$= \lim_{x \to 0} e^{-\alpha(x-x_0)^2} \int dx_0 \frac{2\alpha x_0}{\sqrt{\alpha^2 x_0^2}} e^{-ikx}$$

or $\alpha = -\frac{ik}{2x_0}$ or $x_0 = -\frac{i k}{2\alpha}$
Thus:
\[
I = \lim_{\alpha \to 0} \int_{-\infty}^{\infty} e^{-\alpha (x-x_0)^2} \, dx \, e^{\alpha x_0^2}
\]

But \[
\int_{-\infty}^{\infty} e^{-\alpha (x-x_0)^2} \, dx = \sqrt{\frac{\pi}{\alpha}}
\]

Therefore,
\[
I = \frac{1}{2\pi} \sqrt{\frac{\pi}{\alpha}} e^{-\frac{k^2}{4\alpha}}
\]

Let \(4\alpha = \Delta^2\)

\[
\lim_{\Delta \to 0} \frac{1}{\sqrt{\pi \Delta^2}} \exp \left( -\frac{k^2}{4\Delta^2} \right) = \delta(k) \quad Q.E.D.
\]

Remark: There are eigenfunctions of \(K\) with complex eigenvalues, but then \(K\) is not hermitian: the value of terms at the boundary, which we have been throwing out, are not actually zero. So consider only \(K\) such that eigenvalues are real. (Sounds circular, but is not, as discussed in Shankar.)
Fourier transform in bra-ket notation

Let $|f\rangle$ be a function on the infinite interval $[-\infty, +\infty]$ with $\langle x | f \rangle = f(x)$.

Then $\langle k | f \rangle = \int_{-\infty}^{\infty} \langle k | x \rangle \langle x | f \rangle \, dx$

$\langle k | x \rangle = \langle x | k \rangle^* = \frac{1}{\sqrt{2\pi}} e^{-ikx}$

So $f(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x) \, dx$

Similarly

$f(x) = \langle x | f \rangle = \int_{-\infty}^{\infty} \langle x | k \rangle \langle k | f \rangle \, dk$

assuming $\int_{-\infty}^{\infty} |k| |k| \, dk = 1$

$\langle x | k \rangle = \langle k | x \rangle^* = \frac{1}{\sqrt{2\pi}} e^{ikx}$

So $f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} f(k) \, dk$
The $x$'s and $k$'s are equally good bases for the $SU$ complex functions on $[-\infty, +\infty]$.

More matrix elements

$$<k' | k | k'> = k' \delta(k - k')$$

What about the operator $X$?

$X$ is the operator defined by the condition

$$X |x\rangle = x |x\rangle$$

Hence

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

How about $<f | x | f>$?

$$<f | x | f> = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} <f | x | x'> <x' | x | f>$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) x' \delta(x - x') f(x')$$

$$= \int_{-\infty}^{\infty} f(x) x f(x)$$

(Expectation value of $x$

in the basis $|f\rangle$.)
\[ \langle k' | x | k \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx \, dx' \, e^{-i k x - i k' x'} \langle k' | x | k \rangle \\
= \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \, e^{-i k x - i k' x'} \delta(x - x') \\
= \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \, e^{-i k x} \int_{-\infty}^{\infty} dx' \, e^{i k' x'} \\
= \frac{1}{2\pi} i \frac{d}{dk'} \int_{-\infty}^{\infty} dx \, e^{-i (k - k') x} \\
= -\delta(k - k') \\
= +\frac{1}{2\pi} i \frac{d}{dk} \delta(k - k') = \frac{1}{2\pi} i \delta'(k - k') \]

**Commutator of \( X \) and \( K \):**

We have \( X | f \rangle = x | f \rangle \)

which means

\[ X | f \rangle = \int_{-\infty}^{\infty} x \, f(x) | x \rangle \, dx \]

\[ = \int_{-\infty}^{\infty} x \, f(x) | x \rangle \, dx = | x f \rangle \text{ by definition} \]

Likewise: \( K | f \rangle = | x f \rangle \) by definition

\[ = \int_{-\infty}^{\infty} \frac{df}{dx} | x \rangle \, dx \]
Then \( X |s\rangle = -i X |\frac{df}{dx}\rangle = x - i \frac{df}{dx} |s\rangle \)

\( K X |s\rangle = K |x s\rangle = i \left( \frac{d}{dx} (x |s\rangle) \right) \)

\( = -i |f + x \frac{df}{dx}\rangle \)

Therefore,

\( (XK - KX) |s\rangle = \left[ x, K \right] |s\rangle = \left[ i, \frac{df}{dx} \right] |s\rangle = -i \frac{df}{dx} |s\rangle \)

\( = i |s\rangle \)

So, since this is true for any \( f \),

we have

\[ \left[ x, K \right] = i \frac{df}{dx} \]

Comment on an equation like

\( K |s\rangle = i |\frac{df}{dx}\rangle \)

We will generally want to take inner products of such operators, e.g.,

\[ \langle f | K | s \rangle = -i \langle f | \frac{df}{dx} \rangle \]

\[ = -i \int \langle f | x \rangle \langle x | \frac{df}{dx} \rangle dx \]

\[ = -i \int \langle f | x \rangle \langle x | \frac{df}{dx} \rangle dx = -i \int f(x) \frac{df}{dx} x dx \]
The equation $|\psi\rangle = \int_{-\infty}^{\infty} f(x) |x\rangle \, dx$.

What does it mean?

It means we are expanding a function in the complete basis $|x\rangle$, and that $f(x)$ is like the expansion coefficient.

Hilbert space: a complete vector space in which the vectors can be normalized to unity or to a Dirac delta function.

A side remark: a few theorems on the Dirac delta function.

$\delta(x-a) = 0$ if $x \neq a$.

$\int_{x_1}^{x_2} \delta(x-a) \, dx = \begin{cases} 1 & \text{if } x_1 < a < x_2 \\ 0 & \text{if } a \text{ not in interval} \end{cases}$

$\int_{x_1}^{x_2} f(x) \delta(x-a) \, dx = f(a)$ since $\delta(x-a) = 0$ unless $x = a$. 

$\int_{-\infty}^{\infty} f(x) \delta(x-a) \, dx = f(a)$.
\[ \int_{x_1}^{x_2} f(x) \delta'(x-a) \, dx = \int_{x_1}^{x_2} f(x) \frac{d}{dx} \delta(x-a) \, dx \]
\[ = f(x) \delta(x-a) \bigg|_{x_1}^{x_2} - \int_{x_1}^{x_2} f'(x) \delta(x-a) \, dx \]
\[ = -f'(a) \]

Also, \( \delta(f(x)) = \sum_{i=1}^{m} \frac{\delta(x-x_i)}{|f'(x_i)|} \)

where \( x_i = i^{th} \) zero of \( f(x) \).

[Optional exercise]
Classical Mechanics Review:

Newton's second law in 1D:

\[ F = \frac{dp}{dt} = -\frac{dV}{dx} \quad \text{if } V(x) \text{ is a potential.} \]

\[ p = mv \quad \text{so} \]

\[ m \frac{dv}{dt} = -\frac{dV}{dx} = m \frac{d^2x}{dt^2} \]

This is a second order differential equation in one unknown \( x \), so we need two constants of the motion.

\( \Rightarrow \) Usually, these are taken as initial position and velocity.

An alternative approach starts from the principle of least action. We say that \( x_i \) and \( x_f \) are the initial and final positions and we want to find the path the particle takes to get from \( x_i \) to \( x_f \). According to the principle of least action, the particle takes the
path which minimizes the action $S$ defined by

$$S[x(t)] = \int_{t_i}^{t_f} L(x, \dot{x}) \, dt$$

where $L(x, \dot{x})$ is the Lagrangian.

Nearby path $x_i, t_i$  \rightarrow path of least action $x_f, t_f$.

Choose $x(t)$ so that $S[x(t)] = \text{minimum}$.

Best way to do this is to write

$$\delta S = \text{some change in action due to a small perturbation of path about the one of least action}.$$

$$\delta S[x(t)] = \int_{t_i}^{t_f} \delta L \delta x \, dt$$
\[ = \int_{t_i}^{t_f} \left[ \frac{\partial L}{\partial x} \delta x(t) + \frac{\partial L}{\partial \dot{x}} \delta \dot{x}(t) \right] \, dt \]

Second term may be written

\[ = \int_{t_i}^{t_f} \frac{\partial L}{\partial x} \frac{d}{dt} \delta x(t) \, dt \]

\[ = \left[ \frac{\delta x(t)}{\delta x} \right]_{t_i}^{t_f} - \int_{t_i}^{t_f} \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \delta \dot{x}(t) \right) \, dt \]

Since \( \delta x(t_i) = \delta x(t_f) = 0 \) (fixed initial and final positions)

\[ \delta S = \int_{t_i}^{t_f} \left[ \frac{\partial L}{\partial x} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) \right] \delta x(t) \, dt \]

\[ = 0 \text{ (defined by } \delta x(t) \text{)} \]

Since \( \delta s = 0 \) for any path, \( \) must have

\[ \left[ \right] = 0 \text{ or } \frac{\partial L}{\partial x} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) = 0 \]

Lagrange's equation
In order for this method to give Newton's Law back for the example just given, we may write

\[ L = T - V \]

where \( T = \frac{1}{2} m \dot{x}^2 \) and

\[ V = V(x) \]

Then

\[ \frac{\partial L}{\partial \dot{x}} = -\frac{dV}{dx} \]

\[ \frac{d}{dt} \left( m \dot{x} \right) = m \ddot{x} \]

and eq. of motion becomes

\[ m \ddot{x} = -\frac{dV}{dx} - m\dddot{x} = 0 \]

Hamiltonian Formulation:

Define the momentum

\[ p = \frac{\partial L}{\partial \dot{x}} \]
Then we also introduce a **Hamiltonian function**

\[ \mathcal{H} = \mathcal{L} = \frac{\partial L}{\partial \dot{x}} \dot{p} - L \]

and write \( \mathcal{H} \) in terms of the variables \( p \) and \( x \) instead of \( x \) and \( \dot{x} \).

How does this work for the above example?

Well, we have \( \mathcal{H} = p \dot{x} - \frac{1}{2} m \dot{x}^2 + V(x) \)

Also \( p = \frac{\partial L}{\partial \dot{x}} = m \dot{x} \) so

\[ \dot{x} = \frac{p}{m} \]

and \( \mathcal{H} = \frac{p^2}{2m} - \frac{p^2}{2m} + V(x) = \frac{p^2}{2m} + V(x) \)

How about equations of motion?

One will be \( \dot{x} = \frac{p}{m} = \frac{\partial \mathcal{H}}{\partial p} \)

The other is \( \dot{p} = -\frac{dV}{dx} = -\frac{\partial \mathcal{H}}{\partial x} \)

These will give back our original eqs. of motion:
\[
\frac{\partial H}{\partial p} = \frac{p}{m} = \dot{v}
\]

and
\[
-\frac{\partial H}{\partial x} = -\frac{\partial V}{\partial x} = \dot{p}.
\]

Why does this work (or how do we get this to work in general?)

Let \( L = L(x, \dot{x}) \) (assume time-independent)

Equation of motion is
\[
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = 0
\]

Let \( \frac{\partial L}{\partial \dot{x}} = p \) so \( \dot{p} = \frac{\partial L}{\partial x} \)

Now define \( H = p \dot{x} - L(x, \dot{x}) \)

\[
\frac{\partial H}{\partial p} = \frac{\partial}{\partial p} \left[ p \dot{x} - L(x, \dot{x}) \right] = \dot{x} + p \frac{\partial \dot{x}}{\partial p} - \frac{\partial L}{\partial \dot{x}} \frac{\partial \dot{x}}{\partial p} = \dot{x}
\]

(since we are replacing variable \( x \) by variable \( p \))

\[
\frac{\partial H}{\partial x} = p \frac{\partial \dot{x}}{\partial x} + \frac{\partial L}{\partial x} \frac{\partial \dot{x}}{\partial x} = \frac{\partial L}{\partial \dot{x}} \frac{\partial \dot{x}}{\partial x} = \dot{p}
\]

from Lagrange's eq.
So our Hamiltonian equations of motion are:

\[
p = -\frac{\partial \mathcal{L}}{\partial \dot{x}} \quad \text{with} \quad \mathcal{H} = \mathcal{L} + \mathcal{E}_p \quad \dot{x} - L
\]

\[
\dot{p} = \frac{\partial \mathcal{H}}{\partial \dot{x}}
\]

and \( p = \frac{\partial \mathcal{H}}{\partial \dot{x}} \).

Generalization to many variables:

\[
L = L \left( \{\dot{x}_i\}, \{\dot{x}_i\} \right)
\]

Lagrange equations:

\[
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_i} \right) - \frac{\partial L}{\partial x_i} = 0
\]

\[
\mathcal{H} = \sum_i p_i \dot{x}_i - L
\]

where \( p_i = \frac{\partial L}{\partial \dot{x}_i} \).

\[
\frac{\partial \mathcal{H}}{\partial \dot{x}_i} = \dot{x}_i \quad \frac{\partial \mathcal{H}}{\partial \dot{p}_i} = \dot{p}_i
\]
In general, if
\[ L = T - V \] where \( T \) is quadratic on the \( x_i \)'s,
then
\[ \frac{\partial L}{\partial t} = T + V \]

Theorem: If \( H \) has no explicit time dependence, then
\[ \frac{dH}{dt} = 0 \]

Proof: \[ \frac{dH}{dt} = \sum_{i=1}^{n} \left( \frac{\partial H}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial H}{\partial p_i} \frac{dp_i}{dt} \right) \]
where we are now writing
\[ \frac{\partial}{\partial q_i} \left[ \sum_{i=1}^{n} \frac{\partial H}{\partial q_i} \left( \frac{\partial H}{\partial p_i} \right) + \frac{\partial H}{\partial p_i} \left( \frac{\partial H}{\partial q_i} \right) \right] = 0 \quad \text{QED} \]

"generalized momenta and coordinates"
E.g. harmonic oscillator:

\[ L = T - V = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2 \]

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = m \ddot{x} + kx = 0 \]

\[ \delta L = p \dot{x} - L = m \ddot{x} - L \]

\[ = \frac{1}{2} \frac{p^2}{m} + \frac{1}{2} k x^2 \]

\[ x = \frac{\partial L}{\partial p} = \frac{p}{m} \]

\[ p = -\frac{\partial L}{\partial x} = -kx = m \dot{x} \quad \text{same as above.} \]

"Poisson brackets":

Suppose we have some quantity

\[ \omega = \omega (\{p_i, q_i\}) = f(q, p) \quad \text{state variables} \]

Then

\[ \frac{d\omega}{dt} = \frac{d\omega}{dt} + \left( \frac{\partial \omega}{\partial p_i} \dot{p}_i + \frac{\partial \omega}{\partial q_i} \dot{q}_i \right) \]

\[ = \frac{d\omega}{dt} + \sum \left( \frac{\partial \omega}{\partial q_i} \frac{\partial \omega}{\partial p_i} \right) \]
\[ \frac{dω}{dt} + \{ω, \mathcal{E}\} = \text{Poisson brackets} \]

If \( \omega \) has no explicit time-dependence, then we just get \( \frac{d\omega}{dt} = \{\omega, \mathcal{E}\} \)

Some basic qualitative ideas of quantum mechanics.

Wave-particle duality.
We understand this somewhat if we think of light.

Suppose we send a monochromatic beam through a double slit.

\[ \text{Note that } I(x) = I_1(x) + I_2(x) \text{ where } I_1 \text{ and } I_2 \text{ are the single slit diffraction patterns} \]
Instead, \( I_1(x) = |E_1(x)|^2 \)
\( I_2(x) = |E_2(x)|^2 \)

and \( \text{But } I(x) = |E_1(x) + E_2(x)|^2 \).

There is an interference pattern.
Add amplitudes, not \( \text{intensities.} \)

On the other hand, we also know that light is made up of \( \text{particles called photons.} \)

The smallest quantum of light is one \( \text{photon, of energy } E = h\nu \) where \( \nu \) is the frequency and \( h \) is Planck's const.

So, what happens if beam is very weak?
Individual photons land on the photographic plate with a probability proportional to
\( I(x) = |E_1(x) + E_2(x)|^2 \) on the screen.

What if only one slit is open? Don't get the interference pattern.
So probability distribution is changed.

How to resolve paradox that you change the prob.
Distribution of the intensity by closing a slit even though any given photon goes through only one slit?
Another example: light going through a polarizer (polaroid filter):

\[ E = E_0 (x \cos \theta + y \sin \theta) \]

Experimental observation:

\[ I \propto E^2 \]

Intensity transmitted through filter is

\[ I' = I \cos^2 \theta \] ("Malus's Law").

A "quantum mechanical" interpretation:

Light is made up of quanta of energy \( h \nu \).
Each one either goes through the polarizer or it doesn't.

Prob. of going through is just \( \cos^2 \theta \).

Once the photon goes through, state of beam is changed; it is all polarized (projected onto one of two "eigenstates" of polarizer - the one polarized \( \parallel \) to \( y \)).

Note also that the measurement disturbs the system - system is not the same after we "measure" its polarization.
Note that in order to really ascertain the angle $\theta$ of the original beam, must let lots of photons try to get through.

So much for photons: they have both particle and wave characteristics. (Quantization of light from, e.g., blackbody radiation, photoelectric effect, etc.)

How about material particles and matter waves? Can diffract electron beams, just like light. Let's say we have a particle (a free particle) with energy $E = \frac{p^2}{2m}$.

It too has a wavelength, namely (de Broglie, 1923)

$$\lambda = \frac{h}{|p|}$$

E.g., Davisson-Germer experiment (1927)

E-beam

Electrons have energy $E = \frac{p^2}{2m}$

Therefore, they have wavelength $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$
See scattering of electrons off lattice.

Only at certain angles or energies does one see sharp maxima due to constructive interference.

So the intensity $I \propto \Phi^2 \frac{\psi_i^2}{\lambda}^2$

$\psi_i = \text{analog of electric field scattered from } i\text{th atom.}$

Can use de Broglie relation to calculate angles very accurately.

So, the basic idea is that there is a "wave function" for the particle, analogous to an electric field for 
angle light.

How do we handle case of one electron?

Again, we say that the electron has a certain probability of being scattered into a certain direction. Once more, build up diffraction pattern only with many electrons.

Now, in case of light, $E(x,t)$ satisfies a wave equation — derived from Maxwell’s equations. For matter waves, there is also a wave equation, called the Schrödinger equation, for the wave amplitude.

We will assume it, not derive it.
\[ \frac{dw}{dt} = \{w, \mathcal{F}\}. \]

Postulates of Quantum Mechanics

I. The state of the particle is described by a vector \( |\psi(t)\rangle \) in a Hilbert space.

II. The independent variables \( x \) and \( p \) of classical mechanics are represented by \( x \) and \( p \) vector Hermitian operators.

\[
\begin{align*}
\langle x' | x \rangle & = \delta(x-x') \\
\langle x' | p \rangle & = -i\hbar \delta'(x-x')
\end{align*}
\]
For some function \( \omega \) of the classical variables \( x \) and \( p \), quantum mechanics replaces this function by an operator function

\[
\mathcal{S}_\omega(x, p) = \omega(x \rightarrow x, p \rightarrow p)
\]

**III.** If the particle is in a state \( |\psi\rangle \), measurement of the variable corresponding to \( \mathcal{S}_\omega \) will yield one of the eigenvalues \( \omega \) with probability

\[
P(\omega) = |\langle \omega | \psi \rangle|^2
\]

As a result of the measurement, the state of the system changes from \( |\psi\rangle \) to \( |\omega\rangle \). As a result of the measurement, the state vector \( |\psi(t)\rangle \) obeys the Schrödinger equation

\[
\frac{i\hbar}{\Delta t} |\psi(t)\rangle = H |\psi(t)\rangle
\]

where \( H \) is the Hamiltonian, constructed from the classical Hamiltonian by the substitutions

\[
p \rightarrow p_\omega \quad x \rightarrow x.
\]

The easiest way to understand this set of postulates is just to apply it to many, many problems.
What is the meaning of the state? Suppose we are considering a particle on 1d. Then the natural basis for the state $|\Psi\rangle$ is with the $x$-basis.

What is the meaning of $|\langle x | \Psi \rangle|^2 = |\Psi(x)|^2$? This gives the probability density of finding the particle at point $x$.

Since the particle must be found somewhere,

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = 1$$

Similarly, the probability density of finding the particle to have momentum $p$ is

$$|\langle p | \Psi \rangle|^2 = |\Psi(p)|^2 \quad \text{with} \quad \int_{-\infty}^{\infty} |\Psi(p)|^2 \, dp = 1$$

Now we already showed that

$$\langle x | A \rangle = \langle x | k \rangle = \frac{1}{\sqrt{2\pi}} e^{-ikx}$$

is an eigenstate of the operator $A$ with eigenvalue $A_k$.

This is also an eigenstate of $P = \hbar k$ with eigenvalue $\hbar k$.

We have to be careful with the normalization, however.
Normalization of $\langle p | x \rangle$

We must have

$$\langle p | x \rangle \propto e^{-i px / \hbar} = Ce^{-i px / \hbar}$$

But we want

$$\int_{-\infty}^{\infty} \langle p | x \rangle \langle x | p' \rangle dx = \langle p | p' \rangle = \delta(p-p')$$

Therefore

$$I = \left| c \right|^2 \int_{-\infty}^{\infty} e^{-i(p-p')x / \hbar} dx = \delta(p-p')$$

Let $\xi = x / \hbar \Rightarrow dx = \hbar d\xi$ and

$$I = \hbar \left| c \right|^2 \int_{-\infty}^{\infty} e^{-i(p-p')\xi} d\xi$$

$$= 2\pi \hbar \left| c \right|^2 \delta(p-p')$$

So

$$C = \frac{1}{\sqrt{2\pi \hbar}}$$
Thus, we can write

\[\langle p \mid x \rangle = \int _{ - \infty } ^ { \infty } \langle p \mid x \rangle \langle x \mid p \rangle \, dx \]

\[= \int _{ - \infty } ^ { \infty } \frac { 1 } { \sqrt { 2 \pi \hbar } } e^{- \frac { i } { \hbar } p x} \psi (x) \, dx \quad \text{where \ \hbar = \frac { \hbar } { \gamma } }\]

**Expectation values:**

\[\langle x \rangle = \int _{ - \infty } ^ { \infty } x | \psi (x) | ^ { 2 } \, dx\]

**First, what is expectation value of position?**

\[\langle x ^ { 2 \rangle} = \int _{ - \infty } ^ { \infty } x ^ { 2 } | \psi (x) | ^ { 2 } \, dx\]

**Expectation value of momentum:**

\[\langle p \rangle = \int _{ - \infty } ^ { \infty } p | \psi (p) | ^ { 2 } \, dp\]

**How about fluctuations in \( x \) and \( p \)?**

Well,

\[\langle x ^ { 2 \rangle} = \int _{ - \infty } ^ { \infty } x ^ { 2 } | \psi (x) | ^ { 2 } \, dx\]

and

\[\langle p ^ { 2 \rangle} = \int _{ - \infty } ^ { \infty } p ^ { 2 } | \psi (p) | ^ { 2 } \, dp\]

\[\Delta X = \sqrt { \langle x ^ { 2 \rangle} - \langle x \rangle ^ { 2 } } = \sqrt { \langle (x - \langle x \rangle) ^ { 2 } \rangle }\]

\[\Delta P = \sqrt { \langle p ^ { 2 \rangle} - \langle p \rangle ^ { 2 } }\]

**Heisenberg uncertainty principle:**

\[\Delta X \Delta P \geq \frac { \hbar } { 2 }\]

To be proved rigorously later.
This is true for any pair of "canonically conjugate" operators which satisfy
\[ [\hat{p}, \hat{x}] = i \hbar \]

I will not prove this here right now, but outline the procedure.

**Example:** suppose \[ \psi(x) = \frac{1}{\sqrt{\pi \Delta^2}} e^{-\frac{(x-a)^2}{2\Delta^2}} \]

\[ \langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 \, dx 
= \int_{-\infty}^{\infty} x e^{-\frac{(x-a)^2}{\Delta^2}} \, dx / (\pi \Delta^2)^{1/2} 
= a + \frac{\Delta^2}{2} \]

\[ \langle x^2 \rangle = \frac{1}{(\pi \Delta^2)^{1/2}} \int_{-\infty}^{\infty} x^2 e^{-\frac{(x-a)^2}{\Delta^2}} \, dx = a^2 + \frac{\Delta^2}{2} \]

So \[ \Delta x = [a^2 + \frac{\Delta^2}{2} - a^2]^{1/2} = \frac{\Delta}{\sqrt{2}} \]

To get \[ \psi(p) \] we write
\[ \psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-i p x / \hbar} \psi(x) \, dx 
= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-i p x / \hbar} e^{-\frac{(x-a)^2}{\Delta^2}} \, dx \]
\( = \left( \frac{\Delta^2}{\pi \hbar^2} \right)^{1/4} e^{-\frac{\alpha}{\sqrt{\hbar}} - \frac{\alpha^2 \Delta^2}{2\hbar} \Delta} \)

\( \langle p \rangle = \int_{-\infty}^{\infty} p |\psi(p)|^2 dp = 0 \)

\( \langle p^2 \rangle = \int_{-\infty}^{\infty} p^2 |\psi(p)|^2 dp = \frac{\hbar}{\sqrt{\Delta}} \sqrt{\Delta} \)

Therefore \( \Delta x \Delta p = \frac{\hbar}{2} \text{ indept of } \Delta \)

\text{Gaussian wave function is optimal in this sense}

The Schrödinger equation:

\( \text{It is } H|\psi\rangle = i\hbar \frac{d}{dt} |\psi\rangle \)

First, setting up the Schrödinger eq.

Need to know \( H \).

As was said before, \( H \) comes from replacing classical variables with quantum-mechanical operators

\( \text{E.g. Harmonic oscillator in 1d:} \)

\( H = \frac{p^2}{2m} + \frac{1}{2} kx^2 \rightarrow \frac{p^2}{2m} + \frac{1}{2} kx^2 \)
3D Harmonic oscillator

\[ H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \frac{1}{2} \hbar (x^2 + y^2 + z^2) \]

What if \( H \) includes a term like \( \alpha p_x^2 \)?

Then we have to worry about the order. Usual rule is to use symmetrized form

i.e. \( \alpha p_x^2 \rightarrow \frac{\alpha}{2} (p_x^2 + x^2 \rho) \), etc.

---

**General approach to the solution:**

(assume \( H \) is not time-dependent, for the moment)

Well, we have

\[ i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \]

1st order in time \( \Rightarrow \) need one initial condition

Suppose we know \( H \). We can expand \( |\psi(t)\rangle \)

in terms of the eigenstates of \( H \), defined by

\[ H |E\rangle = E |E\rangle \quad E \text{ will be real since } H \text{ is Hermitian} \]

In general \( \sum_{E} |E\rangle \langle E| = I \) so

\[ |\psi(t)\rangle = \sum_{E} |E\rangle \langle E| \psi(t) \rangle \equiv \sum_{E} a_E(t) |E\rangle \]

\( a_E(t) \) are the coefficients of the expansion.