Operators in infinite dimensions

Consider the equation

$$\hat{\Omega}|f\rangle = |\tilde{f}\rangle$$

where $|f\rangle, |\tilde{f}\rangle$ are vectors in this infinite-dimensional vector space discussed above. The matrix elements of this equation in the basis $\{|x\rangle \,|\, a \le x \le b\}$ are

$$\langle x|\hat{\Omega}|f\rangle = \langle x|\hat{\Omega}\hat{I}|f\rangle = \langle x|\hat{\Omega}\left(\int_a^b |x'\rangle\langle x'|dx'\right)|f\rangle$$

$$= \int_a^b \underbrace{\langle x|\Omega|x'\rangle}_{O(x,x')}\langle x'|f\rangle dx' = \langle x|\tilde{f}\rangle$$

or $$\tilde{f}(x) = \int_a^b O(x,x')\, f(x')\, dx'$$

One such operator is the derivative operator:

$$\hat{D}|f\rangle = |\tfrac{df}{dx}\rangle \equiv |f'\rangle$$

In the $|x\rangle$ basis the matrix elements of this equation read

$$f'(x) = \frac{df}{dx}(x) = \int_a^b \langle x|\hat{D}|x'\rangle f(x')\, dx' \equiv \int_a^b D_{xx'} f(x')\, dx'$$

From our discussion of the δ-function we recognize that this means

$$\boxed{D_{xx'} = \langle x|\hat{D}|x'\rangle = \delta'(x-x') = \delta(x-x')\frac{d}{dx'}}$$

So the derivative operator is a matrix in our

∞-dimensional vector space. In the $|x\rangle$-basis, it is diagonal ($\sim\delta(x-x')$), with the operator $\frac{d}{dx'}$ repeated over and over on the diagonal. ($\frac{d}{dx'}$ is not a vector space operator (with a hat over it), just a symbol that operates on functions to return their slope.)

Is $\hat{D}$ Hermitian? If it were Hermitian, its matrix element should satisfy

$$D_{xx'} \overset{?}{=} D^*_{x'x}$$

But this is not the case: $D_{xx'} = \delta'(x-x')$ while

$$D^*_{x'x} = \delta'(x'-x)^* = \delta'(x'-x) = -\delta'(x-x')$$

So $\hat{D}$ is anti-Hermitian. To render it Hermitian we can multiply by, say, $-i$:

$$\boxed{\hat{K} = -i\hat{D}}$$

$\hat{K}$ satisfies

$$K^*_{x'x} = \left[-i\delta'(x'-x)\right]^* = i\delta'(x'-x) = -i\delta'(x-x') = K_{xx'}$$

Still, this does not guarantee Hermiticity of $\hat{K}$. To see the problem consider 2 functions $f(x)$, $g(x)$ on $[a,b]$, representing the components of kets $|f\rangle$ and $|g\rangle$ in our vector space when using the $|x\rangle$-basis. For $\hat{K}$ to be Hermitian, it must satisfy

$$\langle g|\hat{K}|f\rangle = \langle g|\hat{K}f\rangle = \langle Kf|g\rangle^* = \langle f|K^+|g\rangle^* = \langle f|\hat{K}|g\rangle^*$$

So we ask

$$\int_a^b\int_a^b \langle g|x\rangle\langle x|\hat{K}|x'\rangle\langle x'|f\rangle\,dx\,dx' \stackrel{?}{=} \left(\int_a^b\int_a^b \langle f|x\rangle\langle x|\hat{K}|x'\rangle\langle x'|g\rangle\,dx\,dx'\right)^* ?$$

$$\Rightarrow \int_a^b dx\, g^*(x)\left(-i f'(x)\right) \stackrel{?}{=} \left[\int_a^b dx\, f^*(x)\left(-i g'(x)\right)\right]^* = i\int_a^b \frac{dg^*}{dx} f(x)\,dx$$

Integrating the l.h.s. by parts gives

$$-i g^*(x) f(x)\Big|_a^b + i\int_a^b \frac{dg^*}{dx} f(x)\,dx$$

So $\hat{K}$ is Hermitian only if the surface term vanishes:

$$g^*(b)f(b) = g^*(a)f(a)$$

This is a marked contrast to the finite dimensional case, where the property $K_{xx'} = K^*_{x'x}$ of the matrix elements was sufficient for Hermiticity. One also needs to look at the behavior of the functions at the end points a and b. $\hat{K}$ is Hermitian if and only if the functions satisfy

$$g^*(b)f(b) = g^*(a)f(a) \quad \forall\, g, f$$

One such set of functions are the configurations $f(x)$ of the string clamped at $x=0, L$. Another example are functions in 3-d space of r, ϑ, φ. For these functions to be single valued, we require $f(\phi+2\pi) = f(\phi)$ (i.e. periodicity in the azimuthal angle). In the space of such periodic fcts, $\hat{K} = -i\frac{d}{d\varphi}$ is a Hermitian operator:

$$g^*(2\pi)f(2\pi) = g^*(0)f(0).$$

In quantum mechanics, we will be interested in functions on all of $\mathbb{R}^3$, i.e. $-\infty \leq x, y, z \leq \infty$.

Let's focus on the dependence on x. There are two classes of functions of x, those that vanish as $|x| \to \infty$, and those that do not, the latter behaving as e^{ikx} (k real). $\hat{K} = -i\, d/dx$ is Hermitian on the set of functions of the first class. What about the second class:

$$e^{ikx} e^{-ik'x}\Big|_{x=-\infty}^{\infty} \overset{?}{=} 0 \quad ?$$

For $k = k'$ this is fine. But for $k \neq k'$ the answer is unclear since e^{ikx} oscillates and does not approach a well-defined limit as $|x| \to \infty$. So we must supply a prescription that eliminates this ambiguity: We define the limit as $|x| \to \infty$ as the average over a large interval at infinity:

$$\lim_{x\to\infty} e^{ikx} e^{-ik'x} = \lim_{\substack{L\to\infty \\ \Delta\to\infty}} \frac{1}{\Delta}\int_L^{L+\Delta} e^{i(k-k')x}\, dx = 0 \text{ for } k \neq k'$$

(Similarly for $x \to -\infty$).

Let's now discuss the eigenvalue problem of $\hat{K} = -i\hat{D}$. This looks hard: how do you find the roots of an infinite-order characteristic polynomial ?!! And then construct the infinity of associated eigenvectors (i.e. solve an infinite set of coupled linear equations) ?!!

It turns out to be quite simple. In fact, you have probably done it before!

Let's start with

$$\hat{K}\,|k\rangle = k\,|k\rangle \qquad (k \in \mathbb{R}\text{, since } \hat{K} \text{ is Hermitian.})$$

We write down the matrix elements in the $|x\rangle$-basis:

$$\langle x|\underset{\uparrow \atop \hat{I}}{\hat{K}}|k\rangle = k\underbrace{\langle x|k\rangle}_{\psi_k(x)} \Rightarrow \int dx'\, \underbrace{K_{xx'}}_{-i\delta(x-x')\frac{d}{dx'}}\,\psi_k(x') = \psi_k(x)$$

$$\Rightarrow -i\frac{d}{dx}\psi_k(x) = k\,\psi_k(x)$$

(We can get here directly by immediately substituting $\hat{K} \to -i\frac{d}{dx}$, its representation in the $|x\rangle$-basis.)

The solution of this differential equation is

$$\langle x|k\rangle = \psi_k(x) = A\,e^{ikx}$$

Normalising the solution yields $A = \frac{1}{\sqrt{2\pi}}$: $\quad |k\rangle \leftrightarrow \frac{e^{ikx}}{\sqrt{2\pi}}$

$$\Rightarrow \langle k|\underset{\uparrow \atop \hat{I}}{}k'\rangle = \int_{-\infty}^{\infty} \langle k|x\rangle\langle x|k'\rangle\,dx' = \int_{-\infty}^{\infty}\frac{dx}{2\pi}\,e^{-i(k-k')x} = \delta(k-k')$$

Since k is a continuous label, we can't normalize $\langle k|k\rangle$ to unity. For operators with continuous eigenvalue spectrum, the convention is to normalize to δ-fcts. with <u>unit weight</u>.

<u>Defn</u>: Vector spaces representing functions like $f(x)$ or e^{ikx} are called <u>Hilbert spaces</u>.

The set of eigenstates $|k\rangle$ diagonalizes $\hat{K}$ [$\langle k|\hat{K}|k'\rangle = k'\langle k|k'\rangle = k'\delta(k-k')$]. Assuming that what holds for finite vector spaces carries over to infinite Hilbert spaces (in fact, this is part of the definition of how to handle the infinity of dimensions in Hilbert space), this set of vectors is complete:

$$\int_{-\infty}^{\infty} dk\, |k\rangle\langle k| = \hat{I}$$

Since the $|k\rangle$ states are orthonormalized, they form a basis (the $\hat{K}$ eigenbasis) of the Hilbert space.
I.e. every vector $|f\rangle \in \mathcal{H} \equiv \mathbb{V}^{\infty}(\mathbb{C})$ can be expanded in the $|k\rangle$ basis, with components

$$f(k) \equiv \langle k|f\rangle = \underset{\substack{\uparrow\\ \hat{I}_x}}{\int_{-\infty}^{\infty}} dx\, \langle k|x\rangle\langle x|f\rangle = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, e^{-ikx} f(x)$$

$\Rightarrow$ $f(k)$ are nothing but the Fourier coefficients of $f(x)$!

Similarly

$$f(x) \equiv \langle x|f\rangle = \underset{\substack{\uparrow\\ \hat{I}_k}}{\int_{-\infty}^{\infty}} dk\, \langle x|k\rangle\langle k|f\rangle = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, e^{ikx} f(k)$$

is the Fourier expansion of $f(x)$. Hence $|f\rangle$ represents the function f in an abstract way, and its components $f(x)$ and $f(k)$ in the $|x\rangle$ and $|k\rangle$ bases represent it in x- and k-space. Just as the $|k\rangle$-states diagonalize $\hat{K}$ [$\hat{K}|k\rangle = k|k\rangle$ and $\langle k|\hat{K}|k'\rangle = k\delta(k-k')$], the $|x\rangle$-states diagonalize $\hat{X}$ [$\hat{X}|x\rangle = x|x\rangle$, $\langle x|\hat{X}|x'\rangle = x\delta(x-x')$] where $\hat{X}$ is the "position operator":

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

$$\Rightarrow \langle x|\hat{X}|f\rangle = \int dx' \langle x|\hat{X}|x'\rangle\langle x'|f\rangle = \int dx'\, x'\,\delta(x-x')\, f(x') = x f(x)$$

$$= \langle x|\tilde{f}\rangle = \tilde{f}(x) \quad \Rightarrow \quad \boxed{\tilde{f}(x) = x f(x)}$$

So $\hat{X}$ acts of a vector $|f\rangle$ (representing the function f) by creating a new vector $|\tilde{f}\rangle$ that, in x-representation, becomes $f(x)$ multiplied by x:

$$\boxed{\langle x|\hat{X}|f\rangle = x\langle x|f\rangle}$$

$\hat{X} = \hat{X}^{+}$ is Hermitian:

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

Similarly $\boxed{\langle k|\hat{K}|f\rangle = k\langle k|f\rangle}$

Just as $\hat{K}$ acts as a derivative $-i\frac{d}{dx}$ in the x-basis,

$$\langle x|\hat{K}|x'\rangle = -i\delta'(x-x') = -i\,\delta(x-x')\frac{d}{dx'}$$

$\hat{X}$ acts as a derivative in the k-basis:

$$\langle k|\underset{\uparrow \atop \hat{I}_x}{\hat{X}}|k'\rangle = \int dx\, \langle k|x\rangle\, x\, \langle x|k'\rangle = \int \frac{dx}{2\pi} x e^{-i(k-k')x}$$

$$= -i\frac{d}{dk'}\int\frac{dx}{2\pi}e^{i(k'-k)x} = -i\frac{d}{dk'}\delta(k'-k) = -i\delta'(k'-k)$$

$$= +i\delta'(k-k')$$

$$\Rightarrow \boxed{\langle k|\hat{X}|k'\rangle = +i\delta'(k-k') = i\,\delta(k-k')\frac{d}{dk'}}$$

It follows that

$$\langle k|\underset{\uparrow \atop \hat{I}_k}{\hat{X}}|f\rangle = \int dk' \langle k|\hat{X}|k'\rangle\langle k'|f\rangle = i\int dk'\,\delta(k-k')\frac{d}{dk'}f(k')$$

$$= i\frac{df(k)}{dk} = i\frac{d}{dk}\langle k|f\rangle$$

Summary:

$$i\frac{d}{dk}f(k) \xleftrightarrow[\text{k-basis}]{} \hat{X}|f\rangle \xleftrightarrow[\text{x-basis}]{} x f(x), \quad f(x) = \langle x|f\rangle$$

$$f(k) = \langle k|f\rangle, \quad k f(k) \longleftrightarrow \hat{K}|f\rangle \longleftrightarrow -i\frac{d}{dx}f(x)$$

$\hat{X}$ and $\hat{K}$ don't commute:

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

$$= -ix\frac{d}{dx}f(x)$$

$\hat{X} = \hat{X}^{+}$

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

$$= \int dx' \,\delta(x-x')\left(-i\frac{d}{dx'}\left(x' f(x')\right)\right) = -i\frac{d}{dx}\left(x f(x)\right)$$

$$\Rightarrow \boxed{\langle x|[\hat{X},\hat{K}]|f\rangle = i\frac{d}{dx}(xf) - ix\frac{df}{dx} = if(x) = i\langle x|f\rangle}$$

This holds for all $|f\rangle$ and all $\langle x|$:

$$\Rightarrow \boxed{[\hat{X},\hat{K}] = i\hat{I}}$$

Example: A normal mode problem in Hilbert space

Consider the displacement $f(x,t)$ of a string of length L clamped at its ends $x=0$ and $x=L$: $f(0,t)=f(L,t)=0 \ \forall t$.

It obeys the classical E.O.M. (we measure t in length units, $vt \mapsto t$ (v = wave propagation speed))

$$\boxed{\frac{\partial^2 f(x,t)}{\partial t^2} - \frac{\partial^2 f(x,t)}{\partial x^2} = 0} \qquad (*)$$

We assume that at $t=0$ the displacement is $f(x,0)$ and the velocity $\dot{f}(x,0) \equiv \frac{\partial f}{\partial t}(x,0) = 0$.

Solve for $f(x,t)$!

We identify $f(x,t)$ as the $|x\rangle$-basis components of a time-dependent vector $|f(t)\rangle$ in Hilbert space. Then $-\frac{\partial^2}{\partial x^2} f(x,t)$ are the x-space components of the vector $\hat{K}^2 |f(t)\rangle$, and $\frac{\partial^2}{\partial t^2} f(x,t)$ are the x-space components of $\frac{d^2}{dt^2}|f(t)\rangle$.

The wave eqn. $(*)$ thus becomes the x-representation of the time-dependent evolution equation

$$\boxed{\frac{d^2}{dt^2}|f(t)\rangle + \hat{K}^2 |f(t)\rangle = 0}. \qquad (**)$$

We solve it with our 3-step weight-loss program:

(1) Solve the eigenvalue problem of $\hat{K}^2$

(2) Construct the propagator $\hat{U}(t)$ in terms of eigenvalues and eigenvectors

(3) $|f(t)\rangle = \hat{U}(t)\,|f(0)\rangle$.

The eigenvalue equation is

$$\hat{K}^2|f\rangle = k^2|f\rangle$$

Its x-space matrix elements are

$$-\frac{d^2}{dx^2} f_k(x) = k^2 f_k(x)$$

The solutions are $f_k(x) = A\cos(kx) + B\sin(kx)$

(we prefer this over $A'e^{ikx} + B'e^{-ikx}$ since it allows easier implementation of $f(0) = f(L) = 0$.)

Since $f_k(0) = 0 \Rightarrow A = 0$

Since $f_k(L) = 0 \Rightarrow B\sin(kL) = 0 \Rightarrow \boxed{kL = m\pi,\ m = 1, 2, 3, \ldots}$

(otherwise $B = 0$ and $f_k \equiv 0$).

$\Rightarrow$ discrete eigenvalue spectrum!

Negative m values are redundant: $\sin(-x) = -\sin(x)$ correspond to the same vector $|f\rangle$.

Normalized solutions:

$$|m\rangle \leftrightarrow f_m(x) = \sqrt{\frac{2}{L}}\sin\left(m\pi\frac{x}{L}\right) \qquad (\text{real!}) \Rightarrow \boxed{k_m = \frac{m\pi}{L}}$$

Eigenvalues!

$$\langle f_m \underset{\underset{\hat{I}_x}{\uparrow}}{|} f_{m'}\rangle = \int_0^L dx\, f_m(x)\, f_{m'}(x) = \delta_{mm'}$$

The $|m\rangle$ basis diagonalizes $\hat{K}^2$. In the $|m\rangle$-basis Eq. (**) reads

$$\frac{d^2}{dt^2}\langle m|f(t)\rangle = -\left(\frac{m\pi}{L}\right)^2\langle m|f(t)\rangle, \quad m = 1, 2, \ldots$$

With vanishing initial velocities the solution is

$$\boxed{\langle m|f(t)\rangle = \langle m|f(0)\rangle\cos\left(\frac{m\pi}{L}t\right)}$$

$$\Rightarrow \quad \boxed{|f(t)\rangle = \sum_{m=1}^{\infty} |m\rangle\langle m|f(t)\rangle = \sum_{m=1}^{\infty} |m\rangle\langle m|f(0)\rangle \cos(\omega_m t) \quad \left(\omega_m = \frac{m\pi}{L}\right)}$$

or

$$\boxed{\hat{U}(t) = \sum_{m=1}^{\infty} |m\rangle\langle m| \cos(\omega_m t)}$$

The solution $|f(t)\rangle = \hat{U}(t)|f(0)\rangle$ becomes in the x-basis

$$\langle x|f(t)\rangle = f(x,t) = \langle x|\hat{U}(t)|f(0)\rangle = \int_0^L dx' \langle x|\hat{U}(t)|x'\rangle f(x',0)$$

Now

$$\langle x|\hat{U}(t)|x'\rangle = \sum_{m=1}^{\infty} \langle x|m\rangle\langle m|x'\rangle \cos(\omega_m t)$$

$$= \frac{2}{L}\sum_{m=1}^{\infty} \sin\left(\frac{m\pi}{L}x\right) \sin\left(\frac{m\pi}{L}x'\right) \cos(\omega_m t)$$

$$\Rightarrow \quad \boxed{f(x,t) = \frac{2}{L}\sum_{m=1}^{\infty} \sin(k_m x)\cos(\omega_m t) \underbrace{\int_0^L dx' \sin(k_m x') f(x',0)}_{\text{Fourier components } f_{k_m}(0)} \quad \left(k_m = \frac{m\pi}{L}\right)}$$

The m^{th} normal mode oscillates with wavenumber $k_m = \frac{m\pi}{L}$ in space (along the length of the string) and with frequency ω_m in time.