Dimension and basis of vector space

Operator

Any mathematical operation like addition, multiplication, division, differentiation etc. can be represented by certain symbols known as operators. In other words operator $\hat{O}$ is a mathematical operation which operates on a function $f(x)$ and changes the function to another function $g(x)$. This can be represented by as

$$\hat{O} f(x) = g(x) \quad \text{——} (1)$$

For example multiplication by x may be considered as an operator as

$$x(2x+3) = 2x^2 + 3x$$

In operator language when an operator $\hat{O} = x$ operate on a function $f(x) = 2x+3$, it changes the function $f(x)$ to another function $g(x) = 2x^2 + 3x$. Similarly $\frac{d}{dx}$ may be considered as an operator. Say $f(x) = 4x^3 + 2x$ then the operator $\hat{O} = \frac{d}{dx}$ operates on the $f(x) = 4x^2 + 2x$ gives another function $\hat{O} f(x) = \frac{d}{dx}(4x^3 + 2x) = 12x^2 + 2 = g(x)$

In quantum mechanics we know that there are some observables quantities such as energy, momentum, position which are denoted by operators. For example the observation of momentum which is denoted by momentum operator $\hat{p}$, the observation of position which is denoted by position operator $\hat{x}$ etc.

To each type of observation (e.g observation of energy, momentum or position) there exists a set of numbers — which are nothing but the possible results of the observations. We already know from the energy levels of hydrogen atom (Electron energy $= \frac{-13.6}{n^2}$ eV, where n is the principal quantum no. When electron jumps from one orbit to another orbit then either photon is emitted or absorbed with energy

$$E = h\nu = E_2 - E_1 = \frac{Z^2 m e^4}{8h^2\epsilon_0^2}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] = -13.6\, Z^2\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] \text{eV}$$

which can be expressed as

$$E = h\nu = \frac{hc}{\lambda} = \frac{Z^2 m e^4}{8h^2\epsilon_0^2}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

$$\frac{1}{\lambda} = \frac{Z^2 m e^4}{8h^3 c\,\epsilon_0^2}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] = R_H Z^2\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

where $R_H = \frac{m e^4}{8h^3 c\,\epsilon_0^2}$ is called the Rydberg constant)

Commutators of two operators

We define the commutator of two operators $\hat{A}$ and $\hat{B}$ as

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}.$$

In general $[\hat{A}, \hat{B}] \neq 0$ i.e the commutator of two operators is not zero.

Let us show this by taking a simple example. Let $\hat{A} = x$, $\hat{B} = \frac{d}{dx}$. Then for any function $\psi(x)$

$$[A, B]\,\psi(x) = \left[x, \frac{d}{dx}\right]\psi(x) = \left[x\frac{d}{dx} - \frac{d}{dx}(x)\right]\psi(x)$$

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

$$\therefore [A, B] = \left[x, \frac{d}{dx}\right] = -1 \neq 0.$$

An eq^n which determines the commutator of two operators is called a commutation relation.

Similarly suppose $\hat{A}$ and $\hat{B}$ operator represent observation of particular observables say position and momentum.

Suppose the position observable is denoted by the operator $\hat{A} = \hat{x} = x$ and the momentum observable is denoted by the operator $\hat{B} = \hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

Then the commutation relation of $\hat{x}$ and $\hat{p}_x$ is

$$[\hat{x}, \hat{p}_x] = [x, -i\hbar \frac{\partial}{\partial x}]$$

$$\therefore [x, -i\hbar \frac{\partial}{\partial x}] \psi(x)$$

$$= \left(x(-i\hbar \frac{\partial}{\partial x}) + i\hbar \frac{\partial}{\partial x}(x)\right) \psi(x)$$

$$= -i\cancel{\hbar} x \frac{\partial \psi}{\partial x} + i\hbar \frac{\partial x}{\partial x} \psi(x) + i\hbar \cancel{x} \frac{\partial}{\partial x} \psi$$

$$= i\hbar \psi(x)$$

$$\therefore [x, -i\hbar \frac{\partial}{\partial x}] \psi(x) = i\hbar \psi(x)$$

$$\boxed{\therefore [\hat{x}, \hat{p}_x] = i\hbar \neq 0}$$

Eigenvalues and Eigenfunctions

Let $\psi(x)$ be a well-behaved func^n of the state of a system and let this be operated on by the operator $\hat{A}$ such that it satisfies the eq^n.

$$\hat{A}\,\psi(x) = \lambda\,\psi(x) \quad \text{—— (1)}$$

Then we say that the no. λ is an eigenvalue of the operator $\hat{A}$ and the function $\psi(x)$ is an eigenfunction of $\hat{A}$. Eq^n (1) is termed as the eigen value eq^n for the operator $\hat{A}$.

Suppose the operand $\psi(x) = \sin 4x$ and the operator $\hat{A} = -\dfrac{d^2}{dx^2}$

$$\therefore\ \hat{A}\,\psi(x) = -\frac{d^2}{dx^2}\sin 4x = -4\frac{d}{dx}(\cos 4x)$$
$$= +16\sin 4x$$

$$\therefore\ -\frac{d^2}{dx^2}\sin 4x = 16\sin 4x$$

So we can say that 16 is an eigenvalue of the operator $-\dfrac{d^2}{dx^2}$ and $\sin 4x$ is the eigenfunction of the operator $-\dfrac{d^2}{dx^2}$.

The eigenfunc^n of momentum operator $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$

The eigenfunc^{n}s of the momentum operator $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ are found by solving the eq^n.

$$\hat{p}_x\,\psi(x) = -i\hbar\frac{\partial}{\partial x}\psi(x) = p\,\psi(x)$$

$$\text{or, } \frac{d}{dx}\psi(x) = +\frac{ip}{\hbar}\psi(x)$$

⑤

or, $\frac{\partial}{\partial x}\psi(x) - \frac{i}{\hbar} p\,\psi(x) = 0$ — (2) 2

The solution of this eqn. (2) is

$\psi(x) = c\, e^{\frac{i}{\hbar}px}$ where c = normalization const.

This is a plane wave which represents a state of definite momentum p (p is the eigenvalue) and $e^{\frac{i}{\hbar}px}$ are the eigenfunctions. The eigenfunctions represent plane wave states of a free particle of momentum p. The normalized wave functions are $\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{i/\hbar\, px}$.

Calculation of commutators

Example

1. Show that $\left[\hat{H}, \hat{p}\right] = 0$ where $\hat{H}$ = Hamiltonian of the system

$$= \text{Total energy} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$$= \frac{p^2}{2m} + V(x)$$

for free particle $V(x)$ $\therefore \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

and $\hat{p}$ is the momentum operator $= -i\hbar\frac{d}{dx}$

Ans. In quantum mechanics the operator which commutes with Hamiltonian is known as constant of motion. In case of free particle since $P.E = V = 0$ so the Hamiltonian operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

$$\therefore \left[\hat{H}, \hat{p}\right]\psi(x) = \hat{H}\hat{p}\,\psi(x) - \hat{p}\,\hat{H}\,\psi(x)$$

$$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[-i\hbar\frac{d\psi(x)}{dx}\right] - \left(-i\hbar\frac{d}{dx}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}\right)$$

$$= i\frac{\hbar^3}{2m}\cancel{\frac{d^3\psi(x)}{dx^3}} - \frac{i\hbar^3}{2m}\cancel{\frac{d^3\psi(x)}{dx^2}} = 0$$

$\therefore \left[\hat{H}, \hat{p}\right] = 0$ i.e. $\hat{H}$ commutes with $\hat{p}$. So momentum is a constant of motion i.e. conserved.

2. Show that $u(x) = e^{-\frac{1}{2}x^2}$ is an eigenfunction of the operator $\hat{A}\left(x, \frac{\partial}{\partial x}\right) = \left(\frac{\partial^2}{\partial x^2} - x^2\right)$

Ans $\hat{A}\,u(x) = \left(\frac{\partial^2}{\partial x^2} - x^2\right)u(x) = \left(\frac{\partial^2}{\partial x^2} - x^2\right)e^{-\frac{1}{2}x^2}$

$$= \frac{\partial}{\partial x}\left(e^{-\frac{x^2}{2}}\left(-\frac{2x}{2}\right)\right) - x^2 e^{-x^2/2}$$

$$= -x\left(e^{-\frac{x^2}{2}}\right) \cdot \left(-\frac{2x}{2}\right) - e^{-\frac{x^2}{2}}(+1) - x^2 e^{-x^2/2}$$

$$= \cancel{x^2 e^{-\frac{x^2}{2}}} - e^{-x^2/2} - \cancel{x^2 e^{-x^2/2}} = -e^{-x^2/2} = -u(x)$$

$$\hat{A}\, u(x) = \left(\frac{\partial^2}{\partial x^2} - x^2\right) u(x) = -u(x)$$

$\therefore u(x) = e^{-x^2/2}$ is an eigenfunction of the operator $\hat{A}\left(x, \frac{\partial}{\partial x}\right)$ with eigenvalue $= -1$ proved.

3. Establish the operator eq^n

$$\frac{\partial}{\partial x} x^n = n x^{n-1} + x^n \frac{\partial}{\partial x}$$ and show that

$$\left[\frac{\partial}{\partial x}, x^n\right] = n x^{n-1}.$$

Ans. Here the operator is $\hat{A} = \frac{\partial}{\partial x} x^n$

Consider any function $\psi(x)$ on which the operator $\hat{A}$ will operate.

$$\therefore \hat{A}\,\psi(x) = \left(\frac{\partial}{\partial x} x^n\right)\psi(x)$$

$$= n x^{n-1}\psi(x) + x^n \frac{\partial \psi(x)}{\partial x}$$

$$\therefore \hat{A}\,\psi(x) = \left(n x^{n-1} + x^n \frac{\partial}{\partial x}\right)\psi(x)$$

$$\therefore \left(\frac{\partial}{\partial x} x^n\right)\psi(x) = \left(n x^{n-1} + x^n \frac{\partial}{\partial x}\right)\psi(x)$$

$$\therefore \boxed{\frac{\partial}{\partial x} x^n = n x^{n-1} + x^n \frac{\partial}{\partial x}}$$ proved

Now we have to show that $\left[\frac{\partial}{\partial x}, x^n\right] = n x^{n-1}$ (5)

We know the commutator of two operators is

$$\left[\frac{\partial}{\partial x}, x^n\right] = \frac{\partial}{\partial x} x^n - x^n \frac{\partial}{\partial x}$$

$\therefore$ For any function $\psi(x)$

$$\left[\frac{\partial}{\partial x}, x^n\right] \psi(x) = \left(\frac{\partial}{\partial x} x^n - x^n \frac{\partial}{\partial x}\right)\psi(x)$$

$$= n x^{n-1}\psi(x) + \cancel{x^n \frac{\partial \psi(x)}{\partial x}} - \cancel{x^n \frac{\partial}{\partial x}\psi(x)}$$

$$\therefore \left[\frac{\partial}{\partial x}, x^n\right]\psi(x) = n x^{n-1}\psi(x)$$

$$\boxed{\therefore \left[\frac{\partial}{\partial x}, x^n\right] = n x^{n-1}}$$ proved.

4. Verify the operator eq^n $\left(\frac{\partial}{\partial x} + x\right)\left(\frac{\partial}{\partial x} - x\right) = \frac{\partial^2}{\partial x^2} - x^2 - 1$

For any func^n $\psi(x)$ on which the operator $\left(\frac{\partial}{\partial x} + x\right)\left(\frac{\partial}{\partial x} - x\right)$ operates and gives

$$\left(\frac{\partial}{\partial x} + x\right)\left(\frac{\partial}{\partial x} - x\right)\psi(x)$$

$$= \left(\frac{\partial}{\partial x} + x\right)\left(\frac{\partial \psi(x)}{\partial x} - x\psi(x)\right)$$

$$= \frac{\partial^2 \psi(x)}{\partial x^2} - \psi(x)\frac{\partial}{\partial x}(x) - \cancel{x\frac{\partial}{\partial x}\psi(x)} + \cancel{x\frac{\partial \psi(x)}{\partial x}} - x^2\psi(x)$$

$$= \frac{\partial^2 \psi(x)}{\partial x^2} - \psi(x) - x^2\psi(x)$$

$$= \left(\frac{\partial^2}{\partial x^2} - x^2 - 1\right)\psi(x)$$

$$\therefore \left(\frac{\partial}{\partial x} + x\right)\left(\frac{\partial}{\partial x} - x\right)\psi(x) = \left(\frac{\partial^2}{\partial x^2} - x^2 - 1\right)\psi(x)$$

$$\therefore \left(\frac{\partial}{\partial x} + x\right)\left(\frac{\partial}{\partial x} - x\right) = \frac{\partial^2}{\partial x^2} - x^2 - 1$$ proved

Orthogonal and Orthonormal functions (9)

If the product of a function $\psi_1(x)$ and the complex conjugate $\psi_2^*(x)$ of other func^n $\psi_2(x)$ vanishes when integrated w.r.t. x over the interval $a \leq x \leq b$, that if

$$\int_a^b \psi_2^*(x)\,\psi_1(x) \, dx = 0 \quad \text{—} (1)$$

Then $\psi_1(x)$ and $\psi_2(x)$ are said to be mutually orthogonal or simply orthogonal in the interval (a,b).

If

$$\int_a^b \psi_k^*(x)\,\psi_k(x)\, dx = 1 \quad \text{—} (2)$$

then the functions ψ_k are said to be normalized in the interval (a,b). The functions which are orthogonal and also normalized are called orthonormal functions. The relations (1) and (2) expressing orthogonality and normalization can be combined into one eq^n using Kronecker delta symbol δ_{mn}

$$\int \psi_m^*(x)\,\psi_n(x)\, dx = \delta_{mn} \quad \text{—} (3)$$

where $\delta_{mn} = 1$ when $m = n$ and
$= 0$ when $m \neq n$.

Eq^n (3) then expresses the orthonormality of eigenfunc^{n}s $\psi_n(x)$. In case of unnormalized func^n, they are expressed as $c\psi$ where c is the normalization coefficient whose value can be obtained as

$$\int c^* \psi_k^* \, c\, \psi_k \, dx = 1$$

$$\therefore c^2 = \frac{1}{\int \psi_k^* \psi_k \, dx} \quad \text{—} (4)$$

(10)

Now we will discuss the concept of operators, operating on the wave function (or eigenstate) $\psi(r,t)$ and providing information about their eigenvalues. We will also study how to write down the equation of motion which governs space and time development of the wavefunction $\psi(r,t)$.

Measurement process as operator operating on the wave func^n. of a particle having definite Linear momentum

We know that a moving particle may be represented by a single infinitely extended propagating plane wave of well defined wave length λ (so $\Delta\lambda = 0$ or $\Delta p = 0$ because $\lambda = \frac{h}{p}$ gives $\Delta p = \frac{h\Delta\lambda}{\lambda^2}$). In this case the particle is spread throughout the region which means if I ask the question 'where is the particle?', the answer is 'it can be anywhere'. That means the position of the particle is totally uncertain which implies $\Delta x = \infty$. But the ~~plane~~ plane wave representing the particle has well defined single value of its wavelength λ and hence well defined value of the wave vector $k \left(= \frac{2\pi}{\lambda}\right)$. This means the uncertainty in its wave vector $\Delta k = 0$ (ie $\Delta p = \hbar\Delta k = 0$) ie uncertainty in momentum is zero.

Again a particle may even be represented by a narrow wave packet [wave packet represents superposi^n of large no. of plane propagating waves having different wavelengths making $\Delta\lambda$ (or $\Delta\lambda = \frac{h}{\Delta p}$ ie Δp) nonzero and Δx, the width of wave packet zero]. In this case

In this case, the wave packet or the particle has a (1)
very well defined position ξ in space ie $\Delta x = 0$ but
infinite uncertain value of its wave vector k ie
($p = \hbar k$) ie $\Delta k = \infty$ which implies $\Delta p = \infty$). In
each case, the Heisenberg uncertainty principle
($\Delta x \Delta k \geq 1$ or $\Delta x \Delta p_x \geq \hbar/2$) is ~~followed~~ being followed.

In fact Heisenberg uncertainty principle has been
obtained through the measurement process. So we can
conclude that any statement about the value of a
physical quantity of the system (ie, the particle or
the corresponding wave) is equivalent to a measurement
of the physical quantity of the system (ie the particle
or the corresponding wave) with suitable experimental
set up which gives that particular value.

For example, suppose we make a statement like
this 'a particle is moving in $+x$ direction with its
linear momentum having value p. This means if
one measures its linear momentum, it will have
sharply defined value p (or sharply defined value of
$\lambda = \frac{h}{p}$ for de Broglie relation). Further this means
we shall measure the linear momentum p or the
wavelength using a double slit arrangement ($\lambda = \frac{\omega \, d}{D}$)
which gives precise value of λ (or p) but gives
no information about the position of the particle
(ie $\Delta x = \infty$). So in quantum mechanics making a
statement about the value of the physical quantity of a
system is equivalent to an experimental measurement
process of that physical quantity on that system (ie particle
or the corresponding wave)

Let us now consider ~~a~~ ~~again~~ the double slit expt with the beam of mono-energetic electrons. (12)
We can measure the wavelength λ of the electron in the beam by measuring fringe width β of the interference pattern on the screen, the distance d between the two slits and ~~D~~ the distance D between the slit and the screen.

A plane propagating classical wave of wave vector $k \left(= \frac{2\pi}{\lambda}\right)$ and angular frequency $\omega \left(= 2\pi\nu = 2\pi \frac{c}{\lambda} = kc\right)$ propagating in +ve x direction is presented by wave displacement $y(x,t)$ as

$$y(x,t) = A\cos(kx - \omega t) \quad \text{--- (1)}$$

But for the moment, let us consider a plane propagating (electron/matter) wave represented by a complex function

$$\psi(x,t) = Ae^{i(kx-\omega t)} \quad \text{--- (2)}$$

Now let us see what the operator $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ operating on the complex wave funcⁿ $\psi(x,t)$ gives

$$-i\hbar\frac{\partial}{\partial x}\psi(x,t) = -i\hbar\frac{\partial}{\partial x}Ae^{i(kx-\omega t)}$$

$$= (-i\hbar)(ik)Ae^{i(kx-\omega t)} = \hbar k Ae^{i(kx-\omega t)}$$

$$= \hbar k\,\psi(x,t) \quad \text{--- (3)}$$

So the operator $-i\hbar\frac{\partial}{\partial x}$ operating on $\psi(x,t)$ gives $\hbar k$ times $\psi(x,t)$.

Now we know that $\hbar k = p$ (using de Broglie relation) the linear momentum of the particle (electron in the beam). So the operator operating on the wave funcⁿ $\psi(x,t)$ which is representing the moving electron gives the information about the linear momentum

$p(=\hbar k)$ of the electron. Thus we see that (13)
on one hand, doing interference expt. by double slit with electron beam described by the wave func^n. $\psi(x,t) = A e^{i(kx-\omega t)}$ and finding the value of $\lambda \left(=\frac{h}{p}\right)$, or the value of the linear momentum of the electron in the beam is equivalent to doing operator algebra with the operator $-i\hbar\frac{\partial}{\partial x}$ operating on the same wave function $\psi(x,t) = A e^{i(kx-\omega t)}$ and finding the value of wave vector k or the linear momentum $p(=\hbar k)$. So in a way quantum mechanics may be called as <u>operator mechanics</u>.

After studying the role of operator $-i\hbar\frac{\partial}{\partial x}$ on the wave func^n. $\psi(x,t)$, let us see the role of one more operation $i\hbar\frac{\partial}{\partial t} = \hat{H}$. We find

$$E = h\nu = \frac{h}{2\pi}\frac{2\pi\nu}{\omega} = \hbar\omega$$

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = i\hbar\frac{\partial}{\partial t} A e^{i(kx-\omega t)}$$
$$= (i\hbar)(-i\omega) A e^{i(kx-\omega t)} = \hbar\omega\,\psi(x,t)$$
$$= E\,\psi(x,t)$$

where $E=\hbar\omega$ is the energy of the particle which is represented by the plane propagating wave of angular freq. ω. Therefore the operator $i\hbar\frac{\partial}{\partial t}$ when operating on $\psi(x,t)$ gives the value of the energy of the particle.

Thus we have found that when we are dealing with free particles (ie particles propagating with definite, well defined linear momentum) may be written in terms of their wave func^n. $\psi(x,t) = A e^{i(kx-\omega t)}$ and the operators $-i\hbar\frac{\partial}{\partial x}$ and $i\hbar\frac{\partial}{\partial t}$ operating on the wave func^n. $\psi(x,t)$ give the values of linear momentum and energy of the particle respectively

This may be summarized in the table below. (11)

Table 1 : A list of some physical quantities and corresponding operators

Sl. No.	Physical quantity	Corresponding operator
1.	x-component of linear momentum, p_x	$-i\hbar\frac{\partial}{\partial x}$
2.	y - " " " " , p_y	$-i\hbar\frac{\partial}{\partial y}$
3.	z - " " " " , p_z	$-i\hbar\frac{\partial}{\partial z}$
4.	linear momentum p	$-i\hbar\nabla$
5.	kinetic energy $T = \frac{p^2}{2}$	$-\frac{\hbar^2}{2m}\nabla^2$
6.	Energy of the particle E	$i\hbar\frac{\partial}{\partial t}$
7.	Potential energy $V(r,t)$	$V(r,t)$
8.	Total energy $\frac{p^2}{2m}+V(r,t)$	$-\frac{\hbar^2}{2m}\nabla^2+V(r,t)$