Quantum Operators

A quantum state can be represented by a ket vector $|\psi\rangle$, or its Hermitian conjugate (dual vector) $\langle\psi|$, known as a bra vector.

If an operator A maps $|\psi\rangle$ to $|\phi\rangle$,

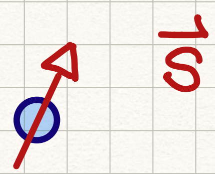
$$|\phi\rangle = A|\psi\rangle \qquad \begin{pmatrix} i \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & i \\ -2i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

its Hermitian conjugate $A^\dagger$ maps $\langle\psi|$ to $\langle\phi|$

$$\langle\phi| = \langle\psi|A^\dagger \qquad (-i \;\; 0) = (0 \;\; 1)\begin{pmatrix} 1 & 2i \\ -i & 0 \end{pmatrix}$$

example

spin-$\frac{1}{2}$ operators



electron

$Q = -e$

$s = \frac{1}{2}$

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Pauli matrices $\sigma_x, \sigma_y, \sigma_z$

It's easy to see that $S_i^\dagger = S_i$ $\quad i = x, y, z$ are Hermitian matrices. It turns out all observables in quantum mechanics can be represented by Hermitian matrices ☺

Let's try to diagonalized S_y.

$$\begin{vmatrix} 0-\lambda & -\frac{i\hbar}{2} \\ \frac{i\hbar}{2} & 0-\lambda \end{vmatrix} = 0 \qquad \lambda^2 - \frac{1}{4}\hbar^2 = 0 \qquad \lambda = \pm\frac{\hbar}{2}$$

Eigenequation $\quad S_y |s_y\rangle = s_y |s_y\rangle$

$$\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \pm\frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}$$

$$-ib = \pm a \quad \longrightarrow \quad b = \pm ia$$

REAL eigenvalues

$$\boxed{\begin{aligned} |s_y = \tfrac{\hbar}{2}\rangle &= \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \\ |s_y = -\tfrac{\hbar}{2}\rangle &= \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} \end{aligned}}$$

orthonormal basis

quantization of spin

$S_y = -\frac{\hbar}{2}, \frac{\hbar}{2}$

Orthonormal Eigenbasis

The Hamiltonian of a quantum system can be represented by a Hermitian matrix $H = H^\dagger$.

Its eigenvalues are energies ☺

$$H|n\rangle = E_n |n\rangle \quad \rightarrow \quad \langle n| H^\dagger = \langle n| \overline{E_n}$$

complex conjugate

Now we would like to show that E_n is real.

$$\langle n|H|n\rangle = E_n \langle n|n\rangle$$

$$\langle n|H^\dagger|n\rangle = \overline{E_n} \langle n|n\rangle$$

$$\rightarrow \quad (E_n - \overline{E_n}) \underbrace{\langle n|n\rangle}_{\text{positive}} = \langle n| \cancel{H - H^\dagger} |n\rangle$$

0

Thus, it leads to the relation $E_n - \overline{E_n} = 0$!

Now we would like to show that

$$\langle n|m\rangle = \delta_{nm} \quad \text{for } E_n \neq E_m$$

The "normalization" part is easy — just rescale the eigenvector so that $\langle n|n\rangle = 1$.

Now, let's work out the "orthogonal" part.

$$H|n\rangle = E_n|n\rangle \rightarrow \langle m|H|n\rangle = E_n\langle m|n\rangle$$

$$\langle m|H = \langle m|E_m \rightarrow \langle m|H|n\rangle = E_m\langle m|n\rangle$$

Upon substraction, it leads to the relation:

$$\underbrace{(E_n - E_m)}_{\text{non-zero}}\langle m|n\rangle = 0 \rightarrow \underbrace{\langle m|n\rangle = 0}_{\text{orthogonal}}$$

Note For $E_n = E_m$ case, the eigenstates $|m\rangle, |n\rangle$ are not necessarily orthogonal. But, for Hermitian matrices, it is always possible to construct $\langle m|n\rangle = 0$ so that the eigenstates form an orthonormal basis!

Commutators

The commutator of two operators A, B is

$$[A,B] = AB - BA$$

If the commutator vanishes, $[A,B]=0$, we call that "A, B commute".

example $[A+B, C] = [A,C] + [B,C]$

The proof is straightforward ~

$$[A+B, C] = (A+B)C - C(A+B)$$
$$= (AC - CA) + (BC - CB)$$
$$= [A,C] + [B,C]$$

example $[AB, C] = A[B,C] + [A,C]B$

$[A, BC] = [A,B]C + B[A,C]$

PROOF:

$$[AB, C] = (AB)C - C(AB)$$
$$= ABC - ACB + ACB - CAB$$
$$= A(BC - CB) + (AC - CA)B$$
$$= A[B,C] + [A,C]B$$

Baker–Campbell–Hausdorff formula

From Wikipedia, the free encyclopedia

In mathematics, the **Baker–Campbell–Hausdorff formula** is the solution for Z to the equation

$$e^X e^Y = e^Z$$

for possibly noncommutative X and Y in the Lie algebra of a Lie group. There are various ways of writing the formula, but all ultimately yield an expression for Z in Lie algebraic terms, that is, as a formal series (not necessarily convergent) in X and Y and iterated commutators thereof. The first few terms of this series are:

$$Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] - \frac{1}{12}[Y,[X,Y]] + \cdots,$$

where "$\cdots$" indicates terms involving higher commutators of X and Y. If X and Y are sufficiently small elements of the Lie algebra $\mathfrak{g}$ of a Lie group G, the series is convergent. Meanwhile, every element g sufficiently close to the identity in G can be expressed as $g = e^X$ for a small X in $\mathfrak{g}$. Thus, we can say that *near the identity* the group multiplication in G—written as $e^X e^Y = e^Z$—can be expressed in purely Lie algebraic terms. The Baker–Campbell–Hausdorff formula can be used to give comparatively simple proofs of deep results in the Lie group–Lie algebra correspondence.

IF $[X,Y]$ commutes with X, Y,

$$[X,[X,Y]] = 0, \qquad [Y,[X,Y]] = 0$$

the BCH formula simplifies,

$$\boxed{e^X e^Y = e^{X+Y+\frac{1}{2}[X,Y]}}$$

Note The exponential operator e^A is defined by its Taylor expansion

$$e^A = \sum_{n=0}^{\infty} \frac{1}{n!} A^n$$

$$= 1 + A + \frac{1}{2!}A^2 + \frac{1}{3!}A^3 + \cdots$$

Momentum Operators

In quantum mechanics, the operators x, p satisfy the canonical commutator,

$$[x, p] = i\hbar \quad \hbar \equiv \frac{h}{2\pi} \; (h\text{-bar})$$

From the commutator, it can be shown that the momentum operator is represented as

$$\boxed{p = -i\hbar \frac{\partial}{\partial x}}$$

Choose $A = x$, $B = \frac{\partial}{\partial x}$ ~

$$[A, B] |\psi\rangle = (AB - BA) |\psi\rangle$$

$$\rightarrow \quad x \frac{\partial}{\partial x} \psi(x) - \frac{\partial}{\partial x} [x \psi(x)]$$

$$= \cancel{x \frac{\partial \psi}{\partial x}} - \psi(x) - \cancel{x \frac{\partial \psi}{\partial x}} = -1 \cdot \psi(x)$$

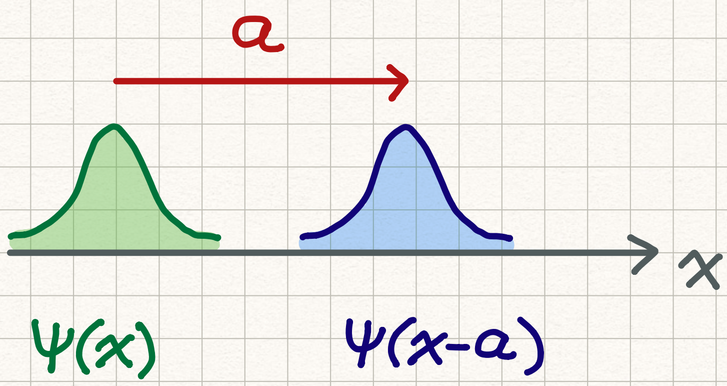
Because $\psi(x)$ is arbitrary,

$$\left[x, \frac{\partial}{\partial x}\right] = -1 \quad \rightarrow \quad \left[x, -i\hbar \frac{\partial}{\partial x}\right] = i\hbar$$

By comparison, the momentum op is $P = -i\hbar \frac{\partial}{\partial x}$

Displacement Operator

Let's study an interesting operator $D(a)$



$$D(a)\,\psi(x) = \psi(x-a)$$

displacement op.

Shift the particle to the right by a.

Making use of Taylor expansion,

$$\psi(x-a) = \psi(x) + \psi'(x)(-a) + \frac{1}{2!}\psi''(x)(-a)^2 + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{(-a)^n}{n!}\left(\frac{\partial}{\partial x}\right)^n \psi(x)$$

the conceptual power of operator

$$= e^{-a\frac{\partial}{\partial x}}\,\psi(x)$$

By comparison, the displacement op. is

$$D(a) = e^{-a\frac{\partial}{\partial x}} = e^{-iap/\hbar}$$

The displacement op. $D(a)$ is related to the momentum op. p :

$$p = i\hbar \left.\frac{dD}{da}\right|_{a=0}$$