Operators in Quantum Mechanics

The mathematical formulation of quantum mechanics (QM) is built upon the concept of an operator. Physical pure states in quantum mechanics are represented as unit-norm vectors (probabilities are normalized to one) in a special complex Hilbert space. Time evolution in this vector space is given by the application of the evolution operator.

Any ***observable***, i.e., any quantity which can be measured in a physical experiment, should be associated with a self-adjoint linear operator. The operators must yield real eigenvalues, since they are values which may come up as the result of the experiment. Mathematically this means the operators must be **Hermitian**. The probability of each eigenvalue is related to the projection of the physical state on the subspace related to that eigenvalue. In the wave mechanics formulation of QM, the wave function varies with space and time, or equivalently momentum and time (see position and momentum space for details), so observables are differential operators.

For example position **x** and momentum **p** are known as a fundamental operators because we can write them as:

$$\hat{x}$$

and $\hat{p}$

$$= -i\hbar \boldsymbol{\nabla}$$

Many operators are constructed from x and p such as Hamiltonian operator $\widehat{\mathrm{H}}$ which is:

$$\widehat{\mathrm{H}} = \frac{p^2}{2m} + \widehat{\mathrm{V}}\,(\hat{x}\,)$$

Which means we can add two operators to get another operator.

Mathematical definition

Operators in quantum mechanics:

Quantum mechanics is a linear theory. According to the principle of superposition, the wave function representing the various states of a physical system can be combined additively and the resulting functions represents new state.

The results obtained from performing a given mathmatical operation upon a wave function ψ is conveniently symbolized by:

$$\varphi = \hat{A}\psi$$

which means the function φ is the result of applying to ψ the operation denoted by $\hat{A}$.

Example: Let $\hat{A} = x$

$\varphi = x\psi$, the function φ resulting from applying the independent variable (x) with ψ. If $\hat{A} = \frac{d}{dx}$, then φ is a derivative of ψ with respect to x. so, $\hat{A}$ is a symbol of mathmatical operation not a multiplication factor of ordinary kind.

$$\frac{d}{dx}(fg) = f\frac{d}{dx}g + \frac{df}{dx}g$$

$$\hat{A}(fg) = f(\hat{A}g) + (\hat{A}f)g$$

where $\hat{A} = \frac{d}{dx}$

Squar operator: squar operator defined as the product of operator with itself.

$$\hat{A}^2 = \hat{A}\hat{A}$$

$$\hat{A}^2 f = \hat{A}(\hat{A}f)$$

if $\hat{A} = \frac{d}{dx}$ then $\frac{d^2}{dx^2}f = \frac{d}{dx}\left(\frac{df}{dx}\right) = \frac{d\bar{f}}{dx} = \bar{\bar{f}}$

Linear Operator

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Linear operator:

The operator $\hat{A}$ is Linear if it satisfies the rules

$$\hat{A}(\psi_1 + \psi_2) = \hat{A}\psi_1 + \hat{A}\psi_2$$

$$\hat{A}(c\psi) = c(\hat{A}\psi)$$

nul or zero operator:

This operator defined by $\hat{O}\psi = 0$ which annihilate the function to which applied.

The identity or unit operator:

$$\hat{1}\psi = \psi$$

produce no changes with operand.

Sum of two operators:

$$\hat{C} = \hat{A} + \hat{B}$$

$$\hat{C}\psi = \hat{A}\psi + \hat{B}\psi$$

product of two operators:

$$\hat{A}(\hat{B}\psi) = \hat{C}\psi$$

$\hat{C}$ is the product of two operators $\hat{A}\hat{B}$

Note: $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ may not equal

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

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

$$\hat{A} = \frac{d}{dx}, \quad \hat{B} = x$$

Eigen function and eigenvalue

(3)

Example:

Is $\frac{d}{dx}$ linear operator?

ans yes, because it obys the previous rules.

Example: Is $\sqrt{\ }$ a linear operator?

No, because:

$$\sqrt{f(x) + g(x)} \neq \sqrt{f(x)} + \sqrt{g(x)}$$

« Eigenfunctions and eigenvalues »

If $\hat{A}$ is a given operator, the function:

$$\phi = \hat{A}\psi \quad \text{---} (1)$$

which results from applying operator $\hat{A}$ on ψ, will ~~in general~~ in general be linearly independent. However, for some function ψ

$$\hat{A}\psi = \alpha\psi \quad \text{----} (2)$$

If ψ is a member of the classis of physically meaningful functions, it is an eigenfunction of the operator $\hat{A}$. The number (α) is called the eigenvalue of $\hat{A}$ associated with the eigenfunction (ψ).

Example 1

e^{2x} is an eigenfunction of operator $\frac{d}{dx}$ with eigenvalue 2

from eq (2) $\frac{d}{dx}(e^{2x}) = 2e^{2x}$

Example 2: Find the eigenfunction and eigenvalues of the operator $\frac{d}{dx}$, if we impose the boundary conditions that the eigenfunctions remain finite for $x \longrightarrow \pm\infty$

solution from equation (2) $\hat{A}\psi = \alpha\psi \Rightarrow \frac{d}{dx}\psi = \alpha\psi \Rightarrow \frac{d\psi}{\psi} = \alpha\, dx$

$\ln\psi = \alpha x + C \Rightarrow \psi = Ce^{\alpha x}$ is the eigenfunction, the eigenvalue is α which can be a number whatever.

Hermitian Operator

In quantum mechanics, operators play a unique role as the observables, i.e. the physical quantities which can be measured, are represented by them. As has already been mentioned previously, it is assumed that the measurement of a physical quantity must yield one of the eigenvalues of the operator representing that physical quantity. Since the observables are always real, the operators representing them should be such that their ***eigenvalues are invariably real***. The Hermitian operators, named after the nineteenth century French mathematician Charles Hermite.

Hermitian operators (4)

physical operator which represents physical quantities are linear operator, but this type of operators should meet an additional requirement which we discuss it now:

An operator $\hat{A}$ that represents the physical property A, the average value

$$A_{exp} = A_{av} = \langle A \rangle = \int \psi^* \hat{A} \psi \, d\tau$$

since $\langle A \rangle$ must be real (because it represents a physical value)

so $\langle A \rangle = \langle A \rangle^*$

and $$\int \psi^* \hat{A} \psi \, d\tau = \int \psi (\hat{A}\psi)^* \, d\tau \quad \text{---- (1)}$$

Eq (1) must hold for any function ψ that represents a possible state of the system.

* A Linear operator that satisfies (1) for all ψ is called Hermitian operator.

As a general case

$$\int f^* \hat{A} g \, d\tau = \int g (\hat{A} f)^* \, d\tau \quad \text{---- (2)}$$

LHS $\hat{A}$ is operator on g

RHS $\hat{A}$ is operator on f

if $g = f$ then equation (2) reduce to (1) we can proof ① by assuming

let $w = f + cg$

$$\int (f+cg)^* \hat{A}(f+cg)\, d\tau = \int (f+cg)[\hat{A}(f+cg)]^* d\tau$$

$$\int (f^* + c^* g^*) \hat{A} f\, d\tau + \int (f^* + c^* g^*) \hat{A} cg\, d\tau = \int (f+g)(Af)^* d\tau$$
$$+ \int (f+cg)(Acg)^* d\tau$$

$$\cancel{\int f^* \hat{A} f d\tau} + c^* \int g^* \hat{A} f\, d\tau + c \int f^* \hat{A} g\, d\tau + \cancel{c^* c \int g^* \hat{A} g\, d\tau} =$$

$$\cancel{\int f (\hat{A} f)^* d\tau} + c \int g (Af)^* d\tau + c^* \int f (\hat{A} g)^* d\tau + \cancel{c c^* \int g (\hat{A} g)^* d\tau}$$

By virtue of ① the 1st and last term should be vanish

$$c^* \int g^* \hat{A} f\, d\tau + c \int f^* \hat{A} g\, d\tau = c \int g (\hat{A} f)^* d\tau + c^* \int f (\hat{A} g)^* d\tau$$

let $c = 1$

$$\int g^* \hat{A} f d\tau + \int f^* \hat{A} g d\tau = \int g (\hat{A} f)^* d\tau + \int f (\hat{A} g)^* d\tau \quad \text{---} ③$$

if $c = i$ and after dividing by i

$$-\int g^* \hat{A} f\, d\tau + \int f^* \hat{A} g\, d\tau = \int g (\hat{A} f)^* d\tau - \int f (\hat{A} g)^* d\tau \quad \text{---} ④$$

Theorem1:

The eigenvalues for Hermitian operators are real.

Add (3) and (4) we get (1)

$$\boxed{\int f^* \hat{A} \hat{g}\, d\tau = \int g\, (\hat{A} f)^*\, d\tau}$$

* The eigen value for Hermitian oprators are real

proof

let ψ is an eigenfunction of $\hat{A}$ with eigen value

$$\hat{A}\psi = a\psi$$

$$\int \psi^* \hat{A}\psi\, d\tau = \int \psi\, (\hat{A}\psi)^*\, d\tau$$

$$\int \psi^* (a\psi)\, d\tau = \int \psi\, (a\psi)^*\, d\tau$$

$$a\int \psi^*\psi\, d\tau = a^*\int \psi\psi^*\, d\tau$$

$$(a - a^*)\int \psi^*\psi\, d\tau = 0$$

since $\int \psi^*\psi\, d\tau \neq 0$

so $(a - a^*) = 0$

$$\boxed{a = a^*}$$

Theorem 2:

The eigenvectors for Hermitian operator are orthogonal.

** The eigen vectors for Hermitian operators are orthogonal.

proof

suppose ψ_a, ψ_b are eigen functions of $\hat{A}$ with eigen values a, b with $a \neq b$.

If $\hat{A}$ is Hermitian

then

$$\int \psi_a^* \hat{A} \psi_b \, d\tau = \int \psi_b (\hat{A} \psi_a)^* d\tau$$

$$b \int \psi_a^* \psi_b \, d\tau = a^* \int \psi_b \psi_a^* \, d\tau$$

from 1st collary $a = a^*$

$$(b-a) \int \psi_a^* \psi_b \, d\tau = 0$$

$b \neq a$ from assumtion, then $\int \psi_a^* \psi_b \, d\tau = 0$

so. ψ_a and ψ_b are orthogonal.

Thank you