Operators

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Operators

Operators: When an operator meets a ket, it produces another ket.
(cf. bra: When a bra meets a ket, it produces a scalar.)

- $\hat{M}|A\rangle = |B\rangle$.

Linear Operators

- $\hat{M}z|A\rangle = z|B\rangle$.
- $\hat{M}(|A\rangle + |B\rangle) = \hat{M}|A\rangle + \hat{M}|B\rangle$.

Matrix Representations

We have two kets and a operator with the following relation:
$|A\rangle = \sum_i a_i|i\rangle$, $|B\rangle = \sum_i b_i|i\rangle$, and

$$\hat{M}|A\rangle = |B\rangle.$$

Then,

$$\sum_i \hat{M} a_i|i\rangle = \sum_i \hat{M}|i\rangle a_i = \sum_i b_i|i\rangle.$$

Applying another basis bra $\langle j|$,

$$\sum_i \langle j|\hat{M}|i\rangle a_i = \sum_i b_i \langle j|i\rangle = \sum_i b_i \delta_{ij} = b_j. \tag{1}$$

Matrix Representations

$$\sum_i \langle j|\hat{M}|i\rangle a_i = b_j.$$

If we represent $\langle j|\hat{M}|i\rangle$ as an element of a matrix,

$$\begin{pmatrix} \langle 1|\hat{M}|1\rangle & \langle 1|\hat{M}|2\rangle & \langle 1|\hat{M}|3\rangle & \cdots \\ \langle 2|\hat{M}|1\rangle & \langle 2|\hat{M}|2\rangle & \langle 2|\hat{M}|3\rangle & \cdots \\ \langle 3|\hat{M}|1\rangle & \langle 3|\hat{M}|2\rangle & \langle 3|\hat{M}|3\rangle & \cdots \\ & \vdots & & \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix}, \tag{2}$$

then the meaning of this operator is transparent.

- Now we accept that as an axiom, all physical observable in quantum mechanics are operators such as $\hat{x}$, $\hat{p}$, $\hat{H}$, and $\hat{L}$.
- In general two matrices do not commute $[A, B] \neq 0$.
- Observable must be real: Hermitian operators.

Hermitian Operators

Observable must be "real" in the "real" world.

- $\langle \Psi | \hat{M} \Psi \rangle = \langle \hat{M} \Psi | \Psi \rangle$.

In quantum mechanics, observable must be Hermitian operators.

- $\langle f | \hat{M} g \rangle = \langle \hat{M} f | g \rangle$ for all f and g.
- $\hat{M} = \hat{M}^{\dagger} = [\hat{M}^{T}]^{*}$
- $m_{ji} = m_{ij}^{*}$
- Transpose (^{T}) and complex conjugate (*)

Charles Hermite
(1822 ~ 1901)

Eigenvalues and Eigenvectors

Eigenvectors $|\lambda\rangle$ are special vectors that are transformed into scalar multiples of themselves after linear transformation,

$$\hat{M}|\lambda\rangle = \lambda|\lambda\rangle, \tag{3}$$

where the complex number λ is their eigenvalue. Discriminate between λ and $|\lambda\rangle$.

Eigenvalues and Eigenvectors

How to obtain eigenvectors and eigenvalues?

1. Start from $\hat{M}|\lambda\rangle = \lambda|\lambda\rangle$
2. $(\hat{M} - \lambda \mathrm{I})|\lambda\rangle = |0\rangle$
3. Assuming $|\lambda\rangle$ is nonzero, solve $\det(\hat{M} - \lambda \mathrm{I})$.
4. Solving the characteristic equation, we obtain eigenvalues of $\hat{M}$.
5. By putting eigenvalues back into the eigenvector equation, we can finally find eigenvectors.

Yes. You have to solve many practice problems of eigenvector equations.

Eigenvalues and Eigenvectors in Quantum Mechanics

Time-independent Schrödinger equation:

$$\hat{H}\psi = E\psi. \tag{4}$$

Thus, in a perspective of linear algebra

- $\hat{H}$: operator
- E_n: eigenvalues
- ψ_n: eigenvectors

Hermitian Operators

- Eigenvalues of a Hermitian operator are always real. They are same as their complex conjugate.
- Two different eigenvectors corresponding two different eigenvalues are orthogonal.
- When two eigenvalues are the same (degeneracy), we can choose two orthogonal eigenvectors (Gram-Schmidt orthogonalization).
- Eigenvectors of a Hermitian operator are a complete set. Any vectors can be decomposed by the sum of eigenvectors.

Real eigenvalues

$$\hat{M}|\lambda\rangle = \lambda|\lambda\rangle,$$
$$\langle\lambda|\hat{M}^\dagger = \langle\lambda|\lambda^*.$$

Suppose that $\hat{M}$ is a Hermitian operator ($\hat{M} = \hat{M}^\dagger$),

$$\hat{M}|\lambda\rangle = \lambda|\lambda\rangle,$$
$$\langle\lambda|\hat{M} = \langle\lambda|\lambda^*.$$

Then, we have (applying $\langle\lambda|$ bra or $|\lambda\rangle$ ket),

$$\langle\lambda|\hat{M}|\lambda\rangle = \lambda\langle\lambda|\lambda\rangle,$$
$$\langle\lambda|\hat{M}|\lambda\rangle = \lambda^*\langle\lambda|\lambda\rangle.$$

Therefore the eigenvalues of a Hermitian operator are real ($\lambda = \lambda^*$).

Orthogonal Eigenvectors

$$\hat{M}|\lambda_1\rangle = \lambda_1|\lambda_1\rangle,$$
$$\hat{M}|\lambda_2\rangle = \lambda_2|\lambda_2\rangle,$$

Since $\hat{M}$ is a Hermitian operator,

$$\langle\lambda_1|\hat{M} = \lambda_1\langle\lambda_1|,$$
$$\hat{M}|\lambda_2\rangle = \lambda_2|\lambda_2\rangle,$$

Then, we have (applying $\langle\lambda_1|$ bra or $|\lambda_2\rangle$ ket),

$$\langle\lambda_1|\hat{M}|\lambda_2\rangle = \lambda_1\langle\lambda_1|\lambda_2\rangle,$$
$$\langle\lambda_1|\hat{M}|\lambda_2\rangle = \lambda_2\langle\lambda_1|\lambda_2\rangle.$$

Finally, we have

$$(\lambda_1 - \lambda_2)\langle\lambda_1|\lambda_2\rangle = 0.$$

Degeneracy and Gram-Schmidt Orthogonalization

If $\lambda_1 = \lambda_2$, we can choose two orthogonal eigenvectors by using Gram-Schmidt orthogonalization. You will prove it (assignment 2).

Eigenvectors Decomposition

When we introduce a set of orthonormal eigenvectors $|i\rangle$, any ket $|A\rangle$ can be represented by a linear combination of the eigenvectors:

$$|A\rangle = \sum_i \alpha_i |i\rangle. \tag{5}$$

Where to go next...

Unitary Operators and Quantum Dynamics.