Hermiticity of operators in Quantum Mechanics

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Wave function and Schrödinger equation

The wave function $\Psi(x,t)$ that describes the quantum mechanics of a particle of mass m moving in a potential $V(x,t)$ satisfies the Schrödinger equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t)$$

Operators

Every observable in quantum mechanics is represented by a linear, Hermitian operator.

$$\hat{x} = x$$

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

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$$\hat{\Omega}\Psi(x) = \omega\Psi(x)$$

Linear operator

$$\hat{A}(a\phi) \equiv a\hat{A}\phi$$

$$\hat{A}(\phi_1 + \phi_2) \equiv \hat{A}\phi_1 + \hat{A}\phi_2$$

$$(\hat{A} + \hat{B})\phi \equiv \hat{A}\phi + \hat{B}\phi$$

$$\hat{A}\hat{B}\phi \equiv \hat{A}(\hat{B}\phi)$$

Hermitian operator

An operator $\hat{\Omega}$, which corresponds to a physical observable Ω, is said to be Hermitian if

$$\int \Phi^* \hat{\Omega} \Psi \, \mathrm{d}x = \int (\hat{\Omega}\Phi)^* \Psi \, \mathrm{d}x$$

Briefer notation

The integrals of pairs of functions:

$$(\Phi, \Psi) = \int \Phi^*(x)\Psi(x)\,\mathrm{d}x$$

For any complex constant *a*:

$$(a\Phi, \Psi) = a^*(\Phi, \Psi)$$

$$(\Phi, a\Psi) = a(\Phi, \Psi)$$

Hermitian operator

Hermitian: $$(\Phi, \hat{\Omega}\Psi) = (\hat{\Omega}\Phi, \Psi)$$

Anti-Hermitian: $$(\Phi, \hat{\Omega}\Psi) = -(\hat{\Omega}\Phi, \Psi)$$

Properties of Hermitian operator

- The expectation value of a Hermitian operator is real.
- The eigenvalues of a Hermitian operator are real.
- The eigenfunctions can be organized to satisfy orthonormality.
- The eigenfunctions of Hermitian operator form a complete set of basis functions. Any reasonable wave function can be written as a superposition of eigenfunctions of that operator.

Real expectation value for Hermitian operator

The expectation value of Ω is defined as

$$\langle \Omega \rangle_\Psi = \int \Psi^*(x)\, \hat{\Omega} \Psi(x)\, \mathrm{d}x = (\Psi, \hat{\Omega}\Psi)$$

The complex conjugate

$$(\langle \Omega \rangle_\Psi)^* = \int (\Psi^*\, \hat{\Omega}\Psi)^*\, \mathrm{d}x = \int \Psi(\hat{\Omega}\Psi)^*\, \mathrm{d}x$$

Real expectation value for Hermitian operator

$$
\begin{aligned}
(\langle\Omega\rangle_\Psi)^* &= \int (\hat{\Omega}\Psi)^* \, \Psi \, \mathrm{d}x \\
&= \int \Psi^* \, \hat{\Omega}\Psi \, \mathrm{d}x \\
&= \langle\Omega\rangle_\Psi
\end{aligned}
$$

$$
\begin{aligned}
Z &= A + iB \\
Z^* &= A - iB
\end{aligned}
$$

The expectation value of a Hermitian operator is real.

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Real eigenvalues for Hermitian operator

Assume the operator $\hat{\Omega}$ has an eigenvalue ω associated with a normalized eigenfunction $\Psi(x)$:

$$\hat{\Omega}\Psi(x) = \omega\Psi(x)$$

The expectation value of $\hat{\Omega}$ in the state of $\Psi(x)$:

$$\langle\Omega\rangle_\Psi = (\Psi, \hat{\Omega}\Psi) = (\Psi, \omega\Psi) = \omega(\Psi, \Psi) = \omega$$

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Orthonormal eigenfunctions for Hermitian operator

Assume that the Hermitian operator $\hat{\Omega}$ has a collection of eigenfunctions and eigenvalues:

$$\begin{aligned}
\hat{\Omega}\psi_1(x) &= \omega_1\psi_1(x) \\
\hat{\Omega}\psi_2(x) &= \omega_2\psi_1(x) \\
\hat{\Omega}\psi_3(x) &= \omega_3\psi_1(x) \\
&\vdots
\end{aligned}$$

The list may be finite or infinite.

Orthonormal eigenfunctions for Hermitian operator

$$(\psi_i, \psi_j) = \int \psi_i^*(x)\, \psi_j(x)\, \mathrm{d}x = \delta_{ij}$$

The Kronecker delta: $\delta_{ij} = \begin{cases} 1 & \text{if} \quad i = j, \\ 0 & \text{if} \quad i \neq j. \end{cases}$

Orthonormal eigenfunctions for Hermitian operator

We evaluate $(\psi_i, \hat{\Omega}\psi_j)$ in two different ways.

$$\begin{aligned}(\psi_i, \hat{\Omega}\psi_j) &= (\psi_i, \omega_j\psi_j) \\ &= \omega_j(\psi_i, \psi_j)\end{aligned}$$

$$\omega_i \neq \omega_j$$

$$\begin{aligned}\hat{\Omega}\psi_1(x) &= \omega_1\psi_1(x) \\ \hat{\Omega}\psi_2(x) &= \omega_2\psi_1(x) \\ \hat{\Omega}\psi_3(x) &= \omega_3\psi_1(x) \\ &\vdots\end{aligned}$$

Orthonormal eigenfunctions for Hermitian operator

$$\begin{aligned}(\psi_i,\, \hat{\Omega}\psi_j) &= (\hat{\Omega}\psi_i,\, \psi_j)\\ &= (\omega_i\psi_i,\, \psi_j)\\ &= \omega_i^*(\psi_i,\, \psi_j)\\ &= \omega_i(\psi_i,\, \psi_j)\end{aligned}$$

$$\omega_i \neq \omega_j$$

$$\begin{aligned}\hat{\Omega}\psi_1(x) &= \omega_1\psi_1(x)\\ \hat{\Omega}\psi_2(x) &= \omega_2\psi_1(x)\\ \hat{\Omega}\psi_3(x) &= \omega_3\psi_1(x)\\ &\vdots\end{aligned}$$

Orthonormal eigenfunctions for Hermitian operator

$$(\omega_j - \omega_i)(\psi_i,\ \psi_j) = 0 \quad \Rightarrow \quad (\psi_i,\ \psi_j) = 0$$

$$\boxed{(\psi_i, \psi_j) = \int \psi_i^*(x)\, \psi_j(x)\, \mathrm{d}x = \delta_{ij}}$$

The eigenfunctions of a Hermitian operator can be organized to satisfy orthonormality.

Orthonormal eigenfunctions for Hermitian operator

$$(\psi_i, \psi_j) = \int \psi_i^*(x)\, \psi_j(x)\, \mathrm{d}x = \delta_{ij}$$

It is possible to have degeneracies in the spectrum, namely, different eigenfunctions with the same eigenvalue. In that case one must show that it is possible to choose linear combinations of the degenerate eigenfunctions that are mutually orthogonal.

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A complete set of basis functions for Hermitian operator

The eigenfunctions of $\hat{\Omega}$ form a complete set of basis functions. Any reasonable Ψ can be written as a superposition of eigenfunctions of $\hat{\Omega}$.

$$\Psi(x) = \alpha_1\psi_1(x) + \alpha_2\psi_2(x) + \cdots = \sum_i \alpha_i\psi_i(x)$$

$$\alpha_i = (\psi_i,\ \Psi)$$

A complete set of basis functions for Hermitian operator

$$
\begin{aligned}
(\psi_i,\ \Psi) &= \int \psi_i^*(x)\,\Psi(x) \\
&= \int \psi_i^*(x) \sum_j \alpha_j \psi_j(x)\,\mathrm{d}x \\
&= \sum_j \alpha_j \int \psi_i^*(x)\,\psi_j(x)\,\mathrm{d}x \\
&= \sum_j \alpha_j \delta_{ij} = \alpha_i
\end{aligned}
$$

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