Lecture notes: QM 03

Hermiticity of operators in Quantum Mechanics

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1 Hermitian operator

An operator $\hat{\Omega}$, which corresponds to a physical observable Ω, is said to be Hermitian if (for simplification we shall consider only the one dimensional case which can always be generalized for three dimension and also assume that the wave functions are normalized unless mentioned otherwise)

$$\boxed{\int \Phi^* \hat{\Omega} \Psi \, \mathrm{d}x = \int (\hat{\Omega}\Phi)^* \Psi \, \mathrm{d}x.} \tag{1}$$

We sometimes use a briefer notation for the integrals of pairs of functions:

$$\boxed{(\Phi, \Psi) = \int \Phi^*(x) \Psi(x) \, \mathrm{d}x.} \tag{2}$$

Note that for any complex constant a

$$(a\Phi, \Psi) = a^*(\Phi, \Psi), \qquad (\Phi, a\Psi) = a(\Phi, \Psi). \tag{3}$$

With this notation the condition of Hermiticity is more briefly stated as

$$\boxed{(\Phi, \hat{\Omega}\Psi) = (\hat{\Omega}\Phi, \Psi).} \tag{4}$$

The operator $\hat{\Omega}$ is said to be anti-Hermitian is

$$\boxed{(\Phi, \hat{\Omega}\Psi) = -(\hat{\Omega}\Phi, \Psi).} \tag{5}$$

2 Properties of Hermitian operator

01. The expectation value of a Hermitian operator is real.

The expectation value of Ω is defined as

$$\boxed{\langle\Omega\rangle_\Psi = \int \Psi^*(x)\,\hat{\Omega}\Psi(x)\,\mathrm{d}x = (\Psi, \hat{\Omega}\Psi).} \tag{6}$$

The complex conjugate of the integral is the integral of the complex conjugate of the integrand, therefore

$$(\langle\Omega\rangle_\Psi)^* = \int (\Psi^*\,\hat{\Omega}\Psi)^*\,\mathrm{d}x = \int \Psi(\hat{\Omega}\Psi)^*\,\mathrm{d}x = \int (\hat{\Omega}\Psi)^*\,\Psi\,\mathrm{d}x. \tag{7}$$

Note that $\hat{\Omega}\Psi$ is a wave function, so it makes sense to take its complex conjugate (we never have to think of conjugating $\hat{\Omega}$). Using the Hermiticity of the operator, as defined in (1), we move it into Ψ to get

$$(\langle\Omega\rangle_\Psi)^* = \int \Psi^*\,\hat{\Omega}\Psi\,\mathrm{d}x = \langle\Omega\rangle_\Psi, \tag{8}$$

thus showing that the expectation value is indeed real.

02. The eigenvalues of a Hermitian operator are real.

Assume the operator $\hat{\Omega}$ has an eigenvalue ω_1 associated with a normalized eigenfunction $\psi_1(x)$:

$$\hat{\Omega}\psi_1(x) = \omega_1\psi_1(x). \tag{9}$$

Now compute the expectation value of $\hat{\Omega}$ in the state of ψ_1:

$$\langle\Omega\rangle_{\psi_1} = (\psi_1, \hat{\Omega}\psi_1) = (\psi_1, \omega_1\psi_1) = \omega_1(\psi_1, \psi_1) = \omega_1. \tag{10}$$

Since, the expectation value is real, the eigenvalue ω_1 is also real, as we wanted to show. Note the interesting fact that the expectation value of $\hat{\Omega}$ on an eigenstate is precisely given by the corresponding eigenvalue.

Consider now the collection of eigenfunctions and eigenvalues of the Hermitian operator $\hat{\Omega}$:

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

The list may be finite or infinite.

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

$$(\psi_i, \psi_j) = \int \psi_i^*(x)\, \psi_j(x)\, \mathrm{d}x = \delta_{ij}. \tag{11}$$

For $i = j$, this is just a matter of normalizing properly each eigenfunction, which can easily be done. The equation also states that different eigenfunctions are orthogonal, or have zero overlap. We now explain why this is so for $i \neq j$ with $\omega_i \neq \omega_j$. Indeed, for this we evaluate $(\psi_i,\, \hat{\Omega}\psi_j)$ in two different ways. First

$$(\psi_i,\, \hat{\Omega}\psi_j) = (\psi_i,\, \omega_j\psi_j) = \omega_j(\psi_i,\, \psi_j), \tag{12}$$

and second, using Hermiticity of $\hat{\Omega}$, and the reality of eigenvalues

$$(\psi_i,\, \hat{\Omega}\psi_j) = (\hat{\Omega}\psi_i,\, \psi_j) = (\omega_i\psi_i,\, \psi_j) = \omega_i^*(\psi_i,\, \psi_j) = \omega_i(\psi_i,\, \psi_j). \tag{13}$$

Equating the final right-hand sides in the two evaluations we get

$$(\omega_j - \omega_i)(\psi_i,\, \psi_j) = 0. \tag{14}$$

Since the eigenvalues were assumed different, this proves that $(\psi_i,\, \psi_j) = 0$, as claimed. This is not yet a full proof of (11) because it is possible to have degeneracies in the spectrum, namely, different eigenfunctions with the same eigenvalue. In that case the above argument does not work. One must then show that it is possible to choose linear combinations of the degenerate eigenfunctions that are mutually orthogonal.

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

$$\boxed{\Psi(x) = \alpha_1\psi_1(x) + \alpha_2\psi_2(x) + \cdots = \sum_i \alpha_i\psi_i(x),} \tag{15}$$

with calculable coefficients α_i. Indeed, if we know the eigenfunctions we have that α_i is calculated doing the integral of ψ_i^* against Ψ:

$$\boxed{\alpha_i = (\psi_i,\, \Psi).} \tag{16}$$

We prove this by doing the integral

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

The condition that $\Psi(x)$ is normalized implies a condition on the coefficients α_i. We have

$$\begin{aligned}\int \Psi^*(x)\Psi(x)\,\mathrm{d}x &= \int \sum_i \alpha_i^* \psi_i^*(x) \sum_j \alpha_j \psi_j(x)\,\mathrm{d}x \\ &= \sum_{i,j} \alpha_i^* \alpha_j \int \psi_i^*(x)\psi_j(x)\,\mathrm{d}x \\ &= \sum_{i,j} \alpha_i^* \alpha_j \delta_{ij} = \sum_i \alpha_i^* \alpha_i, \end{aligned} \tag{17}$$

so that the normalization of Ψ implies that

$$\sum_i |\alpha_i|^2 = 1. \tag{18}$$

3 Measurement Postulate

This helps us understanding the way in which Hermitian operators represent observables and learn the rules that they follow.

Postulate: If we measure the Hermitian operator $\hat{\Omega}$ in the state Ψ, the possible outcomes for the measurement are the eigenvalues $\omega_1, \omega_2, \ldots$. The probability p_i to measure ω_i is given by

$$p_i = |\alpha_i|^2, \tag{19}$$

where $\Psi(x) = \sum_i \alpha_i \psi_i(x)$. After the outcome ω_i, the state of the system becomes

$$\Psi(x) = \psi_i(x). \tag{20}$$

This is called the collapse of the wave function.

The collapse of the wave function implies that immediately after the measurement that yielded ω_i a repeated measurement of $\hat{\Omega}$ will yield ω_i with no uncertainty. A small subtlety occurs if we have degenerate eigenstates. Suppose the wave function contains a piece

$$\Psi = (\alpha_i \psi_i + \alpha_k \psi_k) + \ldots \tag{21}$$

where ψ_i and ψ_k happen to have the same eigenvalue ω and the dots represent other terms. Then if we measure ω the state after the measurement collapses to the sum of those two terms

$$\Psi = \frac{\alpha_i \psi_i + \alpha_k \psi_k}{\sqrt{|\alpha_i|^2 + |\alpha_k|^2}}, \tag{22}$$

with the square root denominator included to provide the proper normalization to Ψ. As a consistency check note that the probabilities p_i to find the various eigenvalues as outcomes properly add to one:

$$\sum_i p_i = \sum_i |\alpha_i|^2 = 1 \tag{23}$$

by the normalization condition for Ψ given in (18). The measurement postulate follows the *Copenhagen interpretation* of quantum mechanics.

Note that the measurement postulate uses the property that any vector in a vector space can be written as a sum of different vectors in an infinite number of ways. If we are to measure $\hat{\Omega}_1$ we expand the state in $\hat{\Omega}_1$ eigenstates, if we are to measure $\hat{\Omega}_2$ we expand the state in $\hat{\Omega}_2$ eigenstates, and so on and so forth. Each decomposition is suitable for a particular measurement. Each decomposition reveals the various probabilities for the outcomes of the specific observable.

4 Examples of Hermitian operator

All quantum mechanical operators that correspond to physically observable quantities are Hermitian operators. We shall see some the examples of that here.

01: Position operator $\hat{x}$ is a Hermitian operator.

Proof: Since

$$\begin{aligned}(\Phi,\, \hat{x}\Psi) &= \int \Phi^*(x)\big(\hat{x}\Psi(x)\big)\,\mathrm{d}x \\ &= \int \Phi^*(x)\big(x\Psi(x)\big)\,\mathrm{d}x \\ &= \int \big(x\Phi^*(x)\big)\Psi(x)\,\mathrm{d}x \\ &= \int \big(x\Phi(x)\big)^*\,\Psi(x)\,\mathrm{d}x \\ &= \int \big(\hat{x}\Phi(x)\big)^*\,\Psi(x)\,\mathrm{d}x \\ &= (\hat{x}\Phi,\, \Psi). \end{aligned} \tag{24}$$

From the definition of Hermiticity (4) we conclude that the position operator $\hat{x}$ is a Hermitian operator.

02: Momentum operator $\hat{p}$ is a Hermitian operator.

Proof: We start with $(\Phi,\, \hat{p}\Psi)$ and use $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ to get

$$\begin{aligned}(\Phi,\, \hat{p}\Psi) &= \int \Phi^*(x)\,\big(\hat{p}\Psi(x)\big)\,\mathrm{d}x \\ &= \int \Phi^*(x)\,(-i\hbar)\frac{\partial\Psi(x)}{\partial x}\,\mathrm{d}x \\ &= -i\hbar\int \Phi^*(x)\,\frac{\partial\Psi(x)}{\partial x}\,\mathrm{d}x. \end{aligned}$$

Integrating by parts we have

$$(\Phi,\, \hat{p}\Psi) = -i\hbar\Big[\Phi^*(x)\Psi(x)\Big]_{-\infty}^{\infty} - (-i\hbar)\int \frac{\partial\Phi^*(x)}{\partial x}\,\Psi(x)\,\mathrm{d}x.$$

Since the wave function vanishes as $x \to \pm\infty$ the first term in the right-hand side is zero. Hence

$$\begin{aligned}(\Phi,\, \hat{p}\Psi) &= i\hbar \int \frac{\partial \Phi^*(x)}{\partial x}\, \Psi(x)\, \mathrm{d}x \\ &= \int \left(-i\hbar \frac{\partial \Phi(x)}{\partial x} \right)^* \Psi(x)\, \mathrm{d}x \\ &= \int \big(\hat{p}\Phi(x)\big)^* \,\Psi(x)\, \mathrm{d}x \\ &= (\hat{p}\Phi,\, \Psi). \end{aligned} \tag{25}$$

Therefore, $\hat{p}$ is a Hermitian operator.

Exercise: Show that $\dfrac{\partial}{\partial x}$ is an anti-Hermitian operator while $\dfrac{\partial^2}{\partial x^2}$ is a Hermitian operator.

References

1. Quantum Mechanics by Nouredine Zettili
2. Introduction to Quantum Mechanics by David J. Griffiths
3. Lecture Notes on Quantum Mechanics by Barton Zwiebach, MIT