A short introduction to quantum mechanics IV: the orthogonality of eigenvectors of Hermitian matrices

A Hilbert space is a complex vector space where a state vector (or wave function) lives. In a Hilbert space, matrices called Hermitian matrices play a role similar to that played by symmetric matrices in a real vector space. Hermitian matrices are defined by the condition that the complex conjugate of the Hermitian matrix is equal to the transpose of the Hermitian matrix. Or in other words, a matrix that is self-adjoint is called a Hermitian matrix (adjoint is the combination of both transpose and complex conjugation; an operator or a matrix is called self-adjoint if its adjoint is equal to itself). One remarkable property of a Hermitian matrix is that its eigenvalues are always real. Even though we have already learned this from our earlier article "Eigenvalues and eigenvectors of symmetric matrices and Hermitian matrices," we will prove this again using bra-ket notations. Let $|n\rangle$ be an eigenvector of a Hermitian matrix A with eigenvalue λ_n. In other words,

$$A|n\rangle = \lambda_n|n\rangle \tag{1}$$

Then, we have

$$(A|n\rangle)^\dagger = (\lambda_n|n\rangle)^\dagger \tag{2}$$

which implies

$$\langle n|A^\dagger = \langle n|\lambda_n^* \tag{3}$$

As $A^\dagger = A$, we have

$$\langle n|A = \langle n|\lambda_n^* = \lambda_n^*\langle n| \tag{4}$$

Then, we get:

$$\langle n|A|n\rangle = (\langle n|A)|n\rangle = (\lambda_n^*\langle n|)|n\rangle = \lambda_n^*\langle n|n\rangle \tag{5}$$

Similarly, we get

$$\langle n|A|n\rangle = \langle n|(A|n\rangle) = \langle n|(\lambda_n|n\rangle) = \lambda_n\langle n|n\rangle \tag{6}$$

Therefore we get

$$\lambda_n^*\langle n|n\rangle = \lambda_n\langle n|n\rangle \tag{7}$$

This implies that $\lambda_n^* = \lambda_n$, which means that λ_n is a real number. Therefore we come to the conclusion that the eigenvalues of a Hermitian matrix are always real. This property of Hermitian matrices is very important. In an earlier article, I mentioned that there is a matrix corresponding to any given observable, and the values for a measurement can only be eigenvalues of this matrix. As the values for the measurement must be real, the eigenvalues must also be real. (It doesn't make any sense that the length of this pencil is "$13 + 3i$" centimeters.) Therefore, we can easily see that the matrices corresponding to observables must be Hermitian matrices.

Now, let's prove that all the eigenvectors of a Hermitian matrix are orthogonal to one another. Again, we have proven this before, but we will do this again using bra-ket notation. Let $|n\rangle$ and $|m\rangle$ be eigenvectors of a Hermitain matrix A with eigenvalues λ_n and λ_m. Then, consider $\langle n|A|m\rangle$. We get:

$$\begin{aligned}\langle n|A|m\rangle &= \langle n|A^\dagger|m\rangle = (\langle n|A^\dagger)|m\rangle = (\lambda_n^*\langle n|)|m\rangle \qquad (8)\\ &= \lambda_n^*\langle n|m\rangle = \lambda_n\langle n|m\rangle \qquad (9)\end{aligned}$$

where we have used the fact λ_n is real, as it is an eigenvalue of a Hermitian matrix ($\lambda_n^* = \lambda_n$). Similarly we get

$$\langle n|A|m\rangle = \lambda_m\langle n|m\rangle \qquad (10)$$

Equating these results, we get

$$\lambda_n\langle n|m\rangle = \lambda_m\langle n|m\rangle \qquad (11)$$

implying that $\langle n|m\rangle = 0$ if λ_n is not equal to λ_m. Therefore we have proven that all the eigenvectors of a Hermitian matrix are orthogonal to one another as long as their corresponding eigenvalues are distinct.

This has far-reaching consequences. It implies that we can form an orthogonal basis consisting of eigenvectors of the Hermitian matrices corresponding to observables. (It is known that as long as the eigenvalues are discrete, as opposed to continuous, we can even take the basis to be orthonormal. We will discuss the continuous case later in another article.)

For example letting E_i's be eigenvalues of an Energy matrix, we have an orthonormal basis of $|E_i\rangle$s, that is:

$$\begin{aligned}\langle E_i|E_j\rangle = 0 \quad \text{if} \quad E_i \neq E_j\\ \langle E_i|E_j\rangle = 1 \quad \text{if} \quad E_i = E_j \qquad (12)\end{aligned}$$

(If originally $\langle E_i|E_i\rangle = A$ for some non-zero A, then we can 'normalize' by defining a new eigenvector with the same eigenvalue E_i:

$$|E_i(\text{new})\rangle = \frac{|E_i\rangle}{\sqrt{A}} \qquad (13)$$

It certainly still has the eigenvalue E_i since

$$E|E_i(\text{new})\rangle = E\left(\frac{|E_i\rangle}{\sqrt{A}}\right) = E_i\frac{|E_i\rangle}{\sqrt{A}} = E_i|E_i(\text{new})\rangle \tag{14}$$

Also, its norm is 1, since

$$\langle E_i(\text{new})|E_i(\text{new})\rangle = \frac{\langle E_i|E_i\rangle}{(\sqrt{A})^2} = 1. \tag{15}$$

This is what is meant by 'normalization.'

We can use this orthonormal basis to express an arbitrary vector $|\psi\rangle$ as:

$$|\psi\rangle = \sum_i \psi(E_i)|E_i\rangle \tag{16}$$

This relation can be expressed slightly differently. Recall my article "Dirac's bra-ket notation." The completeness relation takes now in the following form:

$$1 = \sum_i |E_i\rangle\langle E_i| \tag{17}$$

Multiplying by $|\psi\rangle$ on both-hand side, we conclude:

$$|\psi\rangle = \sum_i |E_i\rangle\langle E_i|\psi\rangle = \sum_i \langle E_i|\psi\rangle|E_i\rangle \tag{18}$$

where we used the fact that $\langle E_i|\psi\rangle$ is a just number, so that we just moved it in front of a ket vector. A ket vector multiplied by a number is equal to a number multiplied by a ket vector. So, we have $\psi(E_i) = \langle E_i|\psi\rangle$. Of course, we saw all this in our earlier article "Dirac's bra-ket notation."

Problem 1. As matrices corresponding to observables must be Hermitian matrices, it is known that the position matrices and the momentum matrices are Hermitian. Given this, check whether the following operators are Hermitian.

$$XP_x, \qquad XY, \qquad XP_y, \qquad P_xP_y \tag{19}$$

Summary

- If we have a Hermitian matrix, we can set its eigenvectors to be orthonormal (i.e., orthogonal to each other, and each having the norm 1).