The Unitarity of the time evolution operator

In this article, I will demonstrate that the requirement that the sum of all possible probabilities is 1 implies that the time evolution operator must be unitary. To this end, let's recall what we did earlier. In our first article on quantum mechanics, I noted that a state vector or a wave function can be expressed as follows:

$$|\phi\rangle = \sum_i c_i |i\rangle \tag{1}$$

where $|i\rangle$s are orthonormal eigenvectors of the linear operator corresponding to a certain observable. Then, as I noted, the probability that $|\phi\rangle$ becomes $|i\rangle$ upon observation is given by the following:

$$c_i c_i^* \tag{2}$$

where we have assumed that $|\phi\rangle$ is normalized. (i.e. $\langle\phi|\phi\rangle = 1$)

Since c_i is given by $\langle i|\phi\rangle$, the above expression is equivalent to the following:

$$\langle\phi|i\rangle\langle i|\phi\rangle \tag{3}$$

Given this, the condition that the probabilities sum up to 1 implies the following:

$$1 = \sum_i \langle\phi|i\rangle\langle i|\phi\rangle \tag{4}$$

However, from our earlier article on Dirac's bra-ket notation, we know that the identity operator can be expressed as follows:

$$1 = \sum_i |i\rangle\langle i| \tag{5}$$

Therefore (4) and (5) imply that $\langle\phi|\phi\rangle = 1$. In other words, the condition that the probabilities sum up to 1 is equivalent to the condition that the norm of the normalized wave function is 1, which seems like a tautology since the definition of the normalized wave function is that its norm is 1. However, the following consideration will imply that this is not a simple matter: The wave function evolves along time. The energy of an object changes, the momentum of an object changes, the position of an object changes, and so on. All this implies that the wave function changes. Given this, as we want the sum of the probabilities to always be 1, the wave function that is changing must also satisfy the condition that its norm remains at 1. Let's consider this situation more mathematically. In quantum mechanics, we have the time evolution operator "$U(t)$" defined as follows:

$$|\phi(t)\rangle = U(t)|\phi(0)\rangle \tag{6}$$

where $|\phi(0)\rangle$ is the normalized wave function at time $t = 0$, and $|\phi(t)\rangle$ is the wave function at time t. $U(t)$ is the time evolution operator that sends the wave function at time 0 to time t. Therefore, the condition we want can be put in a mathematical form as follows:

$$1 = \langle\phi(t)|\phi(t)\rangle = \langle\phi(0)|U^{\dagger}(t)U(t)|\phi(0)\rangle \tag{7}$$

As this equation should be satisfied for any arbitrary $|\phi(0)\rangle$ whose norm is 1, we can easily see that the following should also be satisfied:

$$1 = U^{\dagger}(t)U(t) \tag{8}$$

The condition (8) means that the time evolution operator $U(t)$ must be unitary, as a definition of an unitary operator U is the following:

$$1 = U^{\dagger}U \tag{9}$$

This completes the demonstration. We have already encountered the unitarity of the time evolution operator in our earlier article "Information Conservation and the Unitarity of Quantum Mechanics" where we learned that the unitarity of the time evolution operator implies the conservation of information. In this article, we gave another meaning to it: the total probability always sums up to 1.

The Unitarity of the time evolution operator also means that the Hamiltonian operator is Hermitian. Recall that the time-dependent Schrödinger equation can be re-written as

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{10}$$

Now it is easy to see that the solution to the above differential equation is given by following:

$$\psi(x, y, z, t) = e^{-iHt/\hbar}\psi(x, y, z, t = 0) \tag{11}$$

Thus, the time evolution operator is given by

$$U(t) = e^{-iHt/\hbar}. \tag{12}$$

If $U(t)$ is unitary, it should satisfy the following:

$$U^\dagger U = e^{iH^\dagger t/\hbar} e^{-iHt/\hbar} = 1 \tag{13}$$

Thus, if H was not Hermitian, i.e., $H^\dagger \neq H$, the above equation would be violated.

Final comment. Let's say there are n possible states denoted by $|\phi_i(t)\rangle$ with $i = 1, 2, \cdots, n$ where t denotes the time. Then, the transition amplitude from $|\phi_i(t_1)\rangle$ to $|\phi_j(t_2)\rangle$ is defined as

$$\langle \phi_i(t_1) | \phi_j(t_2) \rangle \tag{14}$$

Then, in light of the explanation given earlier in the article, it is easy to see that the probability that ith state at $t = t_1$ changes to jth state at $t = t_2$ is simply given by the square of the magnitude of the transition amplitude. The concept of the transition amplitude will turn out to be useful when we talk about neutrino oscillation in our later article "neutrino oscillation, clarified."

Problem 1. Prove that a product of two unitary matrices is also a unitary matrix.

Summary

- The time evolution operator must be a unitary matrix, as the total probability adds up to 1.