A short introduction to quantum mechanics V: the expectation value of given observable

In this article, we discuss how one can calculate the expectation of given observables supposing that the state vector is known. In our earlier article "Expectation value and standard deviation," I explained how we can calculate the expectation value of something if we know the probability of that thing happens, but let me explain with an example to remind you. The expectation value of an ordinary six sided die can be calculated as follows.

$$\langle \text{Die} \rangle = 1 \times \frac{1}{6} + 2 \times \frac{1}{6} + 3 \times \frac{1}{6} + 4 \times \frac{1}{6} + 5 \times \frac{1}{6} + 6 \times \frac{1}{6} \tag{1}$$

Thus the expectation value can be calculated by summing over the possible values multiplied by their probabilities. Now let's carry this over to quantum mechanics.

Suppose that the state vector is given as follows

$$|\psi\rangle = 0.6|2\text{J}\rangle + 0.8|5\text{J}\rangle \tag{2}$$

where as before $|x\text{J}\rangle$ is the normalized eigenvector of the energy matrix with eigenvalue xJ. (i.e. $\langle x\text{J}|x\text{J}\rangle = 1$) Notice that the state vector $|\psi\rangle$ is also normalized, as:

$$\langle\psi|\psi\rangle = 0.6^2 + 0.8^2 = 1 \tag{3}$$

In physics, we usually assume that a state vector is normalized, because as long as the norm is not infinity we can always normalize it, and because it is convenient and practical to work with normalized vectors.

Given this, from our first article on quantum mechanics, we see that upon observation there is a 0.36 probability that the object's energy is 2J and 0.64 probability that it is 5J. So, the expectation value is

$$\langle E \rangle = 0.6^2 \times 2\text{J} + 0.8^2 \times 5\text{J} = 3.92 \tag{4}$$

However, notice that the same can be calculated as follows:

$$\langle E \rangle = \langle\psi|E|\psi\rangle = (0.6\langle 2\text{J}| + 0.8\langle 5\text{J}|)(2 \times 0.6|2\text{J}\rangle + 5 \times 0.8|5\text{J}\rangle) \tag{5}$$

Therefore, we conclude that the expectation value of E is given by $\langle\psi|E|\psi\rangle$, and similarly for other observables. Notice that while the calculation in (5) is done in the eigenvector basis of E, the expression $\langle\psi|E|\psi\rangle$

is "basis free," so the same answer would be obtained by calculating in any other basis.

Actually, we can show this more rigorously. As before, let

$$|\psi\rangle = \sum_n c_n|\lambda_n\rangle \tag{6}$$

where

$$A|\lambda_n\rangle = \lambda_n|\lambda_n\rangle, \qquad \langle\lambda_n|\lambda_m\rangle = \delta_{nm} \tag{7}$$

Then the probability that we will get value λ_n for A is given by $c_n c_n^*$. Therefore, the expectation value of A is given by

$$\langle A\rangle = \sum_n \lambda_n c_n^* c_n \tag{8}$$

Now, let's calculate $\langle\psi|A|\psi\rangle$ and see if it agrees with the above result. We have

$$\begin{aligned}
\langle\psi|A|\psi\rangle &= \sum_m \langle\lambda_m|c_m^* A \sum_n c_n|\lambda_n\rangle && (9)\\
&= \sum_m \langle\lambda_m|c_m^* \sum_n \lambda_n c_n|\lambda_n\rangle && (10)\\
&= \sum_m \sum_n c_m^* c_n \lambda_n \langle\lambda_m|\lambda_n\rangle && (11)\\
&= \sum_m \sum_n c_m^* \delta_{mn} c_n \lambda_n && (12)\\
&= \sum_n c_n^* c_n \lambda_n && (13)
\end{aligned}$$

This completes the proof. Notice also that the expectation value is always real as long as A is Hermitian; both $c_n^* c_n$ and λ_n are real. It is also easy to see from a slightly different way as follows:

$$\begin{aligned}
(\langle\psi|A|\psi\rangle)^\dagger &= \langle\psi|A^\dagger|\psi\rangle && (14)\\
(\langle\psi|A|\psi\rangle)^* &= \langle\psi|A|\psi\rangle && (15)
\end{aligned}$$

where we used $g^\dagger = g^*$ for a number g and $A^\dagger = A$.

Problem 1. Suppose a system whose Hilbert space is two-dimensional and its orthogonal basis vectors are given by $|A\rangle$ and $|B\rangle$. Now, let's say that a Hermitian operator H acts on these basis vectors as follows:

$$\begin{aligned}
H|A\rangle &= 4|A\rangle - 3i|B\rangle \\
H|B\rangle &= 3i|A\rangle + 2|B\rangle
\end{aligned} \tag{16}$$

Using the following notation,

$$|A\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |B\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{17}$$

express H by a 2×2 matrix, and obtain its expectation value for the case in which the state vector is given by $|A\rangle$.

Summary

- The expectation value of the observable A for the state vector $|v\rangle$ is given by $\langle A\rangle = \langle v|A|v\rangle$.