

Bracket Notation

The formulation of mathematical formulation of quantum mechanics involves numerous integrals. We have already shown that the average energy (or expectation value) for the n th eigenstate of a system can be expressed as

$$\langle E_n \rangle = \frac{\int \Psi_n^* H \Psi_n d\tau}{\int \Psi_n^* \Psi_n d\tau}$$

Integrals of this type are so common and expressions can become so complex that Dirac developed an alternative formulation. In this formulation we can write an integral as a bracket

$$\int \Psi_n^* \Psi_n d\tau = \langle n | n \rangle$$

The significance of the bracket is further that it can be viewed as the inner (or dot) product of two vectors. Thus, it is shorthand notation for a vector space. In the case above, where $|n\rangle$ is a normalized wave function, the inner product is clearly

$$\langle n|n\rangle = 1$$

However, in the general case we may consider two complex vectors A and B , which have an inner product

$$\langle A|B\rangle = A_x^* B_x + A_y^* B_y + A_z^* B_z$$

In this example we have considered a Cartesian space. In this space we could express the vector B in one of two ways:

$$|B\rangle = B_x |e_x\rangle + B_y |e_y\rangle + B_z |e_z\rangle \qquad |B\rangle = \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix}$$

Thus, the inner product can also be expressed as:

$$\langle A|B \rangle = (A_x^* \quad A_y^* \quad A_z^*) \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix}$$

This is scalar multiplication since the result is a scalar.

A linear operator can operate on a ket. For example, the momentum operator is

$$\hat{p}_x |k \rangle = -i\hbar \frac{\partial}{\partial x} |k \rangle$$

Keeping in mind the ket also can represent a wave function, we may consider that this wave function in this instance is:

$$|k \rangle = e^{ikx}$$

In that case our operator equation would give the result.

$$-i\hbar \frac{\partial}{\partial x} |k \rangle = \hbar k |k \rangle$$

Using Operators in the Bracket

The bra or left hand part always signifies that the complex conjugate is to be used. Thus, we do not need to write the star. The wave function is thus written in a more complex notation as

$$\Psi_n = |n \rangle$$

In an operator equation the bracket has the form

$$\int \Psi_n^* H \Psi_n d\tau = \langle n | H | n \rangle$$

An operator O can act either on the ket (from the left) or on the bra (from the right).

$$(\langle n | O) | m \rangle \quad \langle n | (O | m \rangle)$$

When the operator operates from the left it has the complex conjugate form.

We often simply write the quantum numbers of the given wave function in the bra or ket as a shorthand notation. In this way we can represent the wave function of the hydrogen atom as $|n\ell m\rangle$ so that all of the quantum numbers are shown.

The shorthand notation of the bracket has double meaning. It can be used to represent integrals such as the energy given above. However, the bracket is also a dot product, i.e. a projection of one wave function onto another.

When the quantum numbers in the bra equal those in the ket we have the normalization condition. When the quantum numbers are not equal then the bracket is zero if the wave functions are part of an orthonormal set. Since solutions of the Schrodinger equation are part of such a set this fact can be used to prove important theorems of quantum mechanics.

Hermitian Operators

A Hermitian operator is defined by the condition that the operator should be equal to its self-adjoint. For the operator \hat{O} we express this as

$$\hat{O}^\dagger = \hat{O}$$

The self-adjoint is the transpose complex conjugate of a matrix. For a single operator this implies that the operator equation is equal to its complex conjugate,

$$\hat{O}^* \psi^* = \hat{O} \psi$$

Hermitian Operators must have real eigenvalues

The reason that this mathematical statement is important is that it is the key aspect of the proof that the eigenvalue of an operator equation will be real. To see this, we let the eigenvalues of \hat{P} be called p_i and p_j . Then,

$$\langle \psi_i | \hat{P} \psi_j \rangle = p_j \langle \psi_i | \psi_j \rangle \quad \text{and} \quad \langle \hat{P} \psi_i | \psi_j \rangle = p_i^* \langle \psi_i | \psi_j \rangle$$

However, since $\langle \psi_i | \psi_j \rangle = \delta_{ij}$ these will vanish unless $i = j$.

$$p_j = p_j^*$$

which tells us that the eigenvalues are real and that they are identical.

General Normalization

In the general case where a wave function is not normalized we can determine the normalization constant.

The normalization constant N is defined by

$$\Psi = N\psi$$

. To determine N , we can write,

$$\langle \Psi | \Psi \rangle = N^2 \langle \psi | \psi \rangle = 1$$

Therefore,

$$N = \frac{1}{\sqrt{\langle \psi | \psi \rangle}}$$

The normalized wave function is

$$\Psi = \frac{1}{\sqrt{\langle \psi | \psi \rangle}} \psi$$