HERMITIAN OPERATORS

1. Dirac Notation

We first introduce a notation that is due to Dirac. The idea is to reduce notational clutter and give more prominence to the labels identifying the wavefunctions.

In this notation, a **ket** $|n\rangle$ is used for the wavefunction ψ_n. A **bra** $\langle n|$ is used to denote the complex conjugate of the wavefunction, ψ_n^*. A complete *bra-ket* notation, such as $\langle n|n\rangle$ or $\langle n|\hat{Q}|n\rangle$, implies integration over all space. For example, we have

$$\langle n|n\rangle = \int \psi_n^* \psi_n d\tau$$
$$\langle n|\hat{Q}|n\rangle = \int \psi_n^* \hat{Q} \psi_n d\tau$$

2. Hermiticity

Every operator $\hat{Q}$ has a *Hermitian conjugate*, conventionally denoted $\hat{Q}^\dagger$, which has the following property for any two wavefunctions ψ_m and ψ_n satisfying the boundary conditions for the system:

$$\int \psi_m^* \hat{Q} \psi_n d\tau = \int (\hat{Q}^\dagger \psi_m)^* \psi_n d\tau \tag{1}$$

We can write the above using Dirac notation as

$$\langle m| \hat{Q} |n\rangle = \left\langle \hat{Q}^\dagger m \middle| n \right\rangle . \tag{2}$$

An operator is **Hermitian** if it is equal to its Hermitian conjugate, i.e., $\hat{Q} = \hat{Q}^\dagger$, such that Eq. (1) becomes

$$\int \psi_m^* \hat{Q} \psi_n d\tau = \int (\hat{Q} \psi_m)^* \psi_n d\tau \tag{3}$$

We note the following useful properties. If the operator $\hat{Q}$ is Hermitian, then

$$\langle m| \hat{Q} |n\rangle = \int \psi_m^* \hat{Q} \psi_n d\tau = \int (\hat{Q} \psi_m)^* \psi_n d\tau = \left(\int \psi_n^* \hat{Q} \psi_m d\tau \right)^* = \langle n| \hat{Q} |m\rangle^* \tag{4}$$

Similarly,

$$\langle m|n\rangle = \int \psi_m^* \psi_n d\tau = \left(\int \psi_n^* \psi_m d\tau\right)^* = \langle n|m\rangle^* \tag{5}$$

3. Properties of Hermitian operators

Any Hermitian operator has the following properties:

(1) their eigenvalues are always real.
(2) eigenfunctions corresponding to different eigenvalues are orthogonal.

Proof: Suppose we have two eigenfunctions of a Hermitian operator $\hat{Q}$ such that

$$\hat{Q}|m\rangle = q_m |m\rangle \tag{6}$$

$$\hat{Q}|n\rangle = q_n |n\rangle \tag{7}$$

We can pre-multipy Eq. (6) by ψ_n^* and Eq. (7) by ψ_m^*, and integrate over all space to obtain

$$\langle n|\hat{Q}|m\rangle = q_m \langle n|m\rangle \tag{8}$$

$$\langle m|\hat{Q}|n\rangle = q_n \langle m|n\rangle \tag{9}$$

Taking the complex conjugate of Eq. (8), we get

$$\langle n|\hat{Q}|m\rangle^* = q_m^* \langle n|m\rangle^* \tag{10}$$

Now, using the properties in Eqs. (4) and (5), the above becomes

$$\langle m|\hat{Q}|n\rangle = q_m^* \langle m|n\rangle \tag{11}$$

Subtracting the above from Eq. (9), we have

$$0 = (q_n - q_m^*) \langle m|n\rangle \tag{12}$$

We can now deduce the following:

(1) If $m = n$, then $\langle m|n\rangle = \langle n|n\rangle \neq 0$, so that $q_n = q_n^*$, therefore, q_n is real.
(2) If $q_m \neq q_n$, then since both are real, thus $(q_n - q_m^*) \neq 0$, therefore, $\langle m|n\rangle = 0$, i.e., the wavefunctions ψ_m and ψ_n, corresponding to different eigenvalues, are orthogonal.

We can therefore note that in quantum mechanics, any physical property is represented by a Hermitian operator since the measurement of the corresponding physical property must be real. Conversely, if an operator is not Hermitian, it cannot correspond to any physical property as its eigenvalues are not guaranteed to be real.