

Lecture 9: Observability – Hermitic Operators

Giving a general operator \hat{A} it is said to be *hermitic* or *self-adjoint* and is written as

$$\hat{A}^+ = \hat{A}$$

if fulfills the general identity:

$$\int \psi^* (\hat{A}\psi) d\Gamma = \int \psi (\hat{A}\psi)^* d\Gamma = \int (\hat{A}\psi)^* \psi d\Gamma$$

with $d\Gamma$ formally denoting the elementary (space-time) volume of integration.

As a useful illustration let's check the coordinate, momentum and Hamiltonian hermiticity. The position operator is hermitic

$$\hat{x}^+ = \hat{x}$$

because fulfills the successive identities:

$$\int \psi^* \hat{x} \psi dx = \int \psi^* x \psi dx = \int \psi x \psi^* dx = \int \psi (x \psi)^* dx = \int \psi (\hat{x} \psi)^* dx$$

since $x=x^*$ due to its real nature; the momentum operator is as well hermitic

$$\hat{p}_x^+ = \hat{p}_x$$

throughout the identities:

$$\begin{aligned} \int \psi^* \hat{p}_x \psi dx &= \int \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi dx = -i\hbar \int \left[\frac{\partial}{\partial x} (\psi^* \psi) - \psi \frac{\partial}{\partial x} \psi^* \right] dx \\ &= -i\hbar \int \frac{\partial}{\partial x} (\psi^* \psi) dx + \int \psi \left(i\hbar \frac{\partial}{\partial x} \right) \psi^* dx \\ &= -i\hbar \underbrace{\left(\psi^* \psi \right)_{-\infty}^{+\infty}}_0 + \int \psi \left(-i\hbar \frac{\partial}{\partial x} \right)^* \psi^* dx = \int \psi (\hat{p}_x \psi)^* dx \end{aligned}$$

since either direct or conjugate wave-function cancels at infinity; for the squared of momentum operator the hermitic property is even more direct proofed because it is a real operator

$$\hat{p}_x^2 \bullet = \hat{p}_x (\hat{p}_x) \bullet = i\hbar \frac{\partial}{\partial x} \left(i\hbar \frac{\partial}{\partial x} \right) \bullet = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

that automatically fulfills this condition; and the same for all other coordinates; all in all there is clear that the Hamiltonian operator

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}, \hat{y}, \hat{z})$$

as a sum of hermitic operators is an operator as well:

$$\hat{H}^+ = \hat{H}.$$

The hermitic property of Hamiltonian may also directly be checked (or cross-checked) through the following construction; since assuming a prepared normalized state one successively has:

$$\begin{aligned} \partial_t \int \psi^* \psi d\Gamma &= 0 \\ \Leftrightarrow \int (\partial_t \psi^*) \psi d\Gamma + \int \psi^* (\partial_t \psi) d\Gamma &= 0; \end{aligned}$$

However, when considering in the last equality the direct and conjugate variants of temporal Schrödinger equation,

$$\hat{H}\psi = i\hbar \partial_t \psi, \quad (\hat{H}\psi)^* = -i\hbar \partial_t \psi^*,$$

one gets the hermiticity condition for Hamiltonian fulfilled:

$$\int (\hat{H}\psi)^* \psi d\Gamma = \int \psi^* (\hat{H}\psi) d\Gamma.$$

In general, the hermitic property is usually associated with operators that correspond with observables, i.e. providing a unique measured value when applied (operates) on a given (prepared) state characterized by an eigen-function ψ . This can be easily check out by defining the observed value of an operator as its average measure

$$\langle \hat{A} \rangle = \int \psi^* \hat{A} \psi d\Gamma$$

for a (Born) normalized (prepared) eigen-state:

$$1 = \int \psi^* \psi d\Gamma,$$

and then by applying it to calculate its the zero observed dispersion (square of standard deviation). Actually, for observed (average) dispersion one has the value:

$$\begin{aligned}
\langle (\Delta \hat{A})^2 \rangle &= \int \psi^* (\hat{A} - \langle \hat{A} \rangle)^2 \psi d\Gamma \\
&= \int \psi^* (\hat{A} - \langle \hat{A} \rangle) (\hat{A} - \langle \hat{A} \rangle) \psi d\Gamma \\
&= \int [(\hat{A} - \langle \hat{A} \rangle) \psi]^* (\hat{A} - \langle \hat{A} \rangle) \psi d\Gamma \\
&= \int |(\hat{A} - \langle \hat{A} \rangle) \psi|^2 d\Gamma
\end{aligned}$$

that when goes to zero leaves with the eigen-value problem from the hermitic operator:

$$\hat{A}\psi = a_\psi \psi, \quad a_\psi = \langle \hat{A} \rangle_\psi$$

assuring therefore its fully observable character.

Next, worth treating the superposition problem: how eigen-functions of the same operator, having the same eigen-value, i.e. being called *degenerate functions* for degenerate eigen-states, behave if they are considered composed in a linear manner? For better illustration of the answer lets take the two eigen-function case

$$\hat{A}\phi_{1,2} = a\phi_{1,2}$$

producing the superposition wave-function:

$$\psi = c_1\phi_1 + c_2\phi_2, \quad c_{1,2} \in \mathfrak{F}.$$

Then, one can check directly that the eigen-problem is conserved at the superimposed level by the successive determinations:

$$\hat{A}\psi = \hat{A}(c_1\phi_1 + c_2\phi_2) = c_1\hat{A}\phi_1 + c_2\hat{A}\phi_2 = a(c_1\phi_1 + c_2\phi_2) = a\psi$$

supporting the appropriate generalization:

$$\exists \hat{A}\phi_n = a\phi_n, \quad n = \overline{1, g} \Rightarrow \forall \psi_g = \sum_{n=1}^g c_n \phi_n, \quad c_n \in \mathfrak{F} \left| \hat{A}\psi_g = a\psi_g \right.$$

In the same general context, one can say that the eigen-value a is g -fold degenerate if there exist exactly g – linear independent eigen-functions, i.e. having the closure property

$$\sum_{n=1}^g c_n \phi_n = 0 \Leftrightarrow c_1 = c_2 = \dots = c_g = 0,$$

carrying the same eigen-value problem. Then their superposition gives another eigen-function of the same operator, with the same eigen-value; this is the consecration of the so called *superposition principle* in quantum theory.

There eventually remains to unfold the meaning of hermiticity condition for the superposition eigen-function in terms of its g -eigen-components. To this aim, one rewrites the hermiticity expression

$$\int \psi_g^* (\hat{A} \psi_g) d\Gamma = \int (\hat{A} \psi_g)^* \psi_g d\Gamma$$

under its generalized superposition form:

$$\int \sum_{m=1}^g c_m^* \varphi_m^* \left(\hat{A} \sum_{n=1}^g c_n \varphi_n \right) d\Gamma = \int \left(\hat{A} \sum_{m=1}^g c_m \varphi_m \right)^* \sum_{n=1}^g c_n \varphi_n d\Gamma$$

and equivalently as:

$$\sum_{m,n=1}^g c_m^* c_n \left[\int \varphi_m^* (\hat{A} \varphi_n) d\Gamma - \int (\hat{A} \varphi_m)^* \varphi_n d\Gamma \right] = 0$$

from where there follows the generalized hermiticity condition for an operator in terms of its degenerate eigen-functions:

$$\int \varphi_m^* (\hat{A} \varphi_n) d\Gamma = \int (\hat{A} \varphi_m)^* \varphi_n d\Gamma .$$

With these, one may consider the further case in which there are two wave-functions, both as eigen-values of the same hermitic operator, yet producing two different eigen-values:

$$\hat{A} \psi_n = a_n \psi_n, \quad \hat{A} \psi_m = a_m \psi_m, \quad a_n \neq a_m .$$

In these conditions, how we should regard the eigen-functions ψ_n, ψ_m ? The answer is that they have to be *orthogonal*; the proof starts from considering one the above eigen-value problem, say that of ψ_n , multiplied on left by the conjugated of the remaining eigen-function, here ψ_m , integrating the resulted equation over the space-time volume:

$$\int \psi_m^* (\hat{A} \psi_n) d\Gamma = a_n \int \psi_m^* \psi_n d\Gamma ,$$

taking its conjugate (not forget that a_n is a real value):

$$\int \psi_m (\hat{A} \psi_n)^* d\Gamma = a_n \int \psi_m \psi_n^* d\Gamma ,$$

performing the index inversion $m \leftrightarrow n$:

$$\int \psi_n (\hat{A} \psi_m)^* d\Gamma = a_m \int \psi_m^* \psi_n d\Gamma ,$$

using the hermiticity property of the involved operator

$$\int \psi_m^* \hat{A} \psi_n d\Gamma = a_m \int \psi_m^* \psi_n d\Gamma ,$$

and being finally subtracted from the initial one to give:

$$0 = (a_n - a_m) \int \psi_m^* \psi_n d\Gamma ,$$

leaving with the general ortho-normal condition for the eigen-functions belonging to the same hermitic operator:

$$\int \psi_m^* \psi_n d\Gamma = \delta_{mn}$$

in terms of the delta-Kronecker tensor

$$\delta_{mn} = \begin{cases} 1, m = n \\ 0, m \neq n \end{cases}$$

Further use of hermiticity and eigen-value properties are in next employed in obtaining specific quantum theorems.