Lecture 9: Observability – Hermitic Operators

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

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

if fulfills the general identity:

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

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:

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

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

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

throughout the identities:

$$\int \psi^{*}\hat{p}_x \psi dx = \int \psi^{*}\left(-i\hbar\frac{\partial}{\partial x}\right)\psi dx = -i\hbar\int\left[\frac{\partial}{\partial x}\left(\psi^{*}\psi\right) - \psi\frac{\partial}{\partial x}\psi^{*}\right]dx$$

$$= -i\hbar\int\frac{\partial}{\partial x}\left(\psi^{*}\psi\right)dx + \int \psi\left(i\hbar\frac{\partial}{\partial x}\right)\psi^{*} dx$$

$$= -i\hbar\underbrace{\left(\psi^{*}\psi\right)_{-\infty}^{+\infty}}_{0} + \int \psi\left(-i\hbar\frac{\partial}{\partial x}\psi\right)^{*} dx = \int \psi\left(\hat{p}_x\psi\right)^{*} dx$$

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:

$$\partial_t \int \psi^* \psi d\Gamma = 0$$

$$\Leftrightarrow \int (\partial_t \psi^*) \psi d\Gamma + \int \psi^* (\partial_t \psi) d\Gamma = 0\ ;$$

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

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

one gets the hermiticity condition for Hamiltonian fulfilled:

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

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

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

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:

$$\left\langle\left(\Delta\hat{A}\right)^2\right\rangle = \int \psi^*\left(\hat{A}-\left\langle\hat{A}\right\rangle\right)^2 \psi d\Gamma$$

$$= \int \psi^*\left(\hat{A}-\left\langle\hat{A}\right\rangle\right)\left(\hat{A}-\left\langle\hat{A}\right\rangle\right)\psi d\Gamma$$

$$= \int \left[\left(\hat{A}-\left\langle\hat{A}\right\rangle\right)\psi\right]^*\left(\hat{A}-\left\langle\hat{A}\right\rangle\right)\psi d\Gamma$$

$$= \int \left|\left(\hat{A}-\left\langle\hat{A}\right\rangle\right)\psi\right|^2 d\Gamma$$

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

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

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:

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

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

$$\hat{A}\psi = \hat{A}(c_1\varphi_1 + c_2\varphi_2) = c_1\hat{A}\varphi_1 + c_2\hat{A}\varphi_2 = a(c_1\phi_1 + c_2\phi_2) = a\psi$$

supporting the appropriate generalization:

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

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

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

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

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

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:

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

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

$$\int \phi_m^* \left(\hat{A}\varphi_n\right) d\Gamma = \int \left(\hat{A}\phi_m\right)^* \phi_n d\Gamma \ .$$

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:

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

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:

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

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

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

performing the index inversion $m \leftrightarrow n$:

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

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:

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

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.