## 2.9 Expectation Values

If a system is in state $\varphi$ which is not an eigen state of a such operator $\hat{A}$, then it is not possible to say with certainty what measured value will be found for $A$. Therefore, one has to use the average value $\langle A \rangle = \bar{A}$ which called in Q.M. expectation value of $A$. however, it is defined mathematically as;

$$\bar{A} = \langle A \rangle = \frac{\int \psi^* \hat{A} \psi \, d\tau}{\int \psi^* \psi \, d\tau} \qquad \text{...........(2-17)}$$

For a normalized wave function $\varphi$;

$$\bar{A} = \langle A \rangle = \int \psi^* \hat{A} \psi \, d\tau$$

The probability that a measurement leads to the eigen value for such a case is defined as follows;

$$p_n = \frac{|\int \psi_n^* \phi d\tau|^2}{|\int \phi^* \phi d\tau|} \qquad \text{........... (2-18)}$$

For a normalized wave function $\varphi$;

$$p_n = |\int \psi_n^* \phi d\tau|^2$$

**Remark:** The integration in the last mathematical formula is called overlap integral which is a number, that has a value in the range 0 (lowest value) and 1 (maximum value). For the lowest value, the two functions are exactly different while for the maximum value the functions are exactly similar.

We have learned that for each operator $\hat{A}$ there are a set of eigen values $a_n$ ($a_1, a_2, a_3, \ldots$) with corresponding eigen wave functions $\psi_n$ ($\psi_1, \psi_2\, \psi_3$, .....). The not eigen function $\phi$ can be expanded in terms $\psi_n$ as follows;

$$\phi = c_1\psi_1 + c_2\psi_2 + c_3\psi_3 + \text{..........} + c_n\psi_n = \sum_n c_n\psi_n \qquad \text{.........(2-19)}$$

Equation (2-19) called the completeness or linear superposition principle. Since the total probability is unity we can prove the following important relation $\sum_n |c_n|^2 = 1$, as follows;

$$\int_{\text{all space}} \phi^* \phi \, d\tau = 1$$

$$\int \sum_n c_n^* \psi_n^* \cdot \sum_m c_m \psi_m \, d\tau = 1$$

$$\sum_n \sum_m c_n^* c_m \int \psi_n^* \psi_m \, d\tau = 1$$

$$\sum_n \sum_m c_n^* c_m \, \delta_{nm} = 1$$

$$\sum_n c_n^* c_n = 1$$

$$\sum_n |c_n|^2 = 1 \qquad \text{…………(2-20)}$$

Each term in the last equation ($|c_n|^2$) represent the probability that the system being in state $n$. Therefore, the physical meaning of this equation is that the total probability (1) is equal to the partial probabilities ($|c_1|^2 + |c_2|^2 + |c_3|^2 + \cdots$) for the system to be in all of the different states.

On the other hand, each term may have regarded to the probability that a measurement for an observable $A$ leads to the eigen value $a_n$, and can be proved as follows;

$$p_n = |\int \psi_n^* \phi d\tau|^2$$

$$= \left| \int \psi_n^* (c_1\psi_1 + c_2\psi_2 + \cdots) \, d\tau \right|^2$$

$$= \left| c_n \int \psi_n^* \psi_n \, d\tau \right|^2$$

$$= \left| c_n \, \delta_{nn} \right|^2$$

$$p_n = |c_n|^2 \qquad \text{…………(2-21)}$$

Actually, we can prove that the probable results on measure the observable $A$ for a system describe by the non-eigen function $\varphi$, is given by; $\langle A \rangle = \sum_n |c_n|^2 \; a_n$ as follows;

$$\langle A\rangle = \int \phi^* \hat{A}\phi \, d\tau$$
$$= \int \{\sum_n c_n\psi_n\}^* A\{\sum_m c_m\psi_m\} d\tau$$
$$= \int \sum_n c_n^*\psi_n^* \cdot \sum_m c_m A\psi_m d\tau$$
$$= \sum_n c_n^* \sum_m c_m \, a_m \int \psi_n^* \psi_m d\tau$$
$$= \sum_n \sum_m c_n^* c_m \, a_m \, \delta_{nm}$$
$$= \sum_n c_n^* c_n \, a_n$$
$$\langle A\rangle = \sum_n |c_n|^2 \cdot a_n \quad \text{...........(2-22)}$$

This means that the expectation value of $A$ is the sum of each eigen value $a_n$ times the corresponding partial probability $|c_n|^2$ of the system to be in that state $n$.

### 2.11 Variance

The variance defined as the deviation in the measurement result from its expectation value. It is defining by the root-mean-square deviation as follows;

$$\Delta A = \{\langle (A - \langle A\rangle)^2\rangle\}^{1/2} \quad \text{.............. (2-23a)}$$

The last definition can be formulating to another for as follows;

$$(\Delta A)^2 = \langle (A - \langle A\rangle)^2\rangle$$
$$= \int \psi^* (A - \langle A\rangle)^2 \psi \, d\tau$$
$$= \int \psi^* (A^2 - 2A\langle A\rangle + \langle A\rangle^2)\, \psi \, d\tau$$
$$= \int \psi^* A^2 \psi \, d\tau - \int \psi^* (2A\langle A\rangle)\psi \, d\tau + \int \psi^* \langle A\rangle^2 \psi \, d\tau$$
$$(\Delta A)^2 = \langle A^2\rangle - 2\langle A\rangle\langle A\rangle + \langle A\rangle^2$$
$$(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2 \quad \text{.............. (2-23b)}$$

**H.W:** Show that, when a system is describe by an eigen function $\psi_n$, the probability that a measurement for observable *A* yields the value $a_n$ is (1). Find the expectation value of *A* in this case. Calculate the variance in *A*.

### 2.12 Equation of motion and constant of motion

When a wave function $\psi$ is an eigen function for the operator $\hat{A}$ with eigen value *a*. Then all measurements process for the observable *A* leads to the eigen value *a*. i.e. $\langle A \rangle = a$. In this case the observable $A$ is called **constant of motion** (or **conserved**), which means that *A* is time independent quantity. i.e. $\dot{A} = \frac{\partial A}{\partial t} = 0$. Let us try to prove this fact.

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

$$\frac{\partial}{\partial t}\langle A \rangle = \dot{\bar{A}} = \int (\frac{\partial \psi^*}{\partial t} \hat{A} \psi + \psi^* A \frac{\partial \psi}{\partial t}) \; d\tau \qquad \text{………….. (a)}$$

$$\left.\begin{aligned} i\hbar \frac{\partial \psi}{\partial t} &= \hat{H}\psi \\ -i\hbar \frac{\partial \psi^*}{\partial t} &= (\hat{H}\psi)^* \end{aligned}\right\} \qquad \text{…………. (b)}$$

Substitute of equation (b) in equation (a) yields;

$$\dot{\bar{A}} = \int \{ \frac{i}{\hbar} (\hat{H}\psi)^* \hat{A} \psi - \frac{i}{\hbar} \psi^* A \hat{H} \psi \} \; d\tau$$

According to the definition of Hermitian operator we obtain;

$$\int \hat{A}\psi (\hat{H}\psi)^* d\tau = \int \psi^* \hat{H} \, \hat{A} \psi \; d\tau$$

$$\frac{d}{dt}\langle A \rangle = \dot{\bar{A}} = \frac{i}{\hbar} \int \psi^* (\hat{H}\hat{A} - \hat{A}\hat{H}) \; \psi \; d\tau$$

In Q.M we define that;

$$\dot{\bar{A}} = \bar{\dot{A}}$$

$\therefore$

$$\bar{\dot{A}} = \frac{i}{\hbar} \int \psi^* (\hat{H}\hat{A} - \hat{A}\hat{H}) \, \psi \; d\tau \qquad \text{…………….. (2-24)}$$

$$\dot{\hat{A}} = \frac{i}{\hbar} \left[ \hat{H}, \hat{A} \right] \qquad \text{……..…… (2-25)}$$

Equation (25) is called the equation of motion, which imply that an observable $A$ is a constant of motion (conserved) when its operator being commute with the Hamiltonian operator.

**Example**: Show that, the linear momentum $p_x$ of a free particle is a constant of motion.

**Solution:**

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

For a free particle $V(x) = 0$, thus;

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$\dot{\bar{p}} = \frac{i}{\hbar}\left[\hat{H}, \hat{p}\right]$$

$$\dot{\bar{p}} = \frac{i}{\hbar}(\hat{H}\hat{p} - \hat{p}\hat{H})$$

$$\dot{\bar{p}}\psi = \frac{i}{\hbar}(\hat{H}\hat{p} - \hat{p}\hat{H})\psi$$

$$\dot{\bar{p}}\psi = \frac{i}{\hbar}\{(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2})\cdot(-i\hbar\frac{\partial\psi}{\partial x}) - (-i\hbar\frac{\partial}{\partial x})\cdot(\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2})\}$$

$$\dot{\bar{p}}\psi = \frac{i}{\hbar}\{\frac{i\hbar^3}{2m}\frac{\partial^3\psi}{\partial x^3} - \frac{i\hbar^3}{2m}\frac{\partial^3\psi}{\partial x^3}\}$$

$$\dot{\bar{p}} = 0$$

Since, $\dot{\bar{p}} = 0$ thus, $p = \text{constan of motion}$

**Example:** Prove the Ehrenfest theorems that given by; **a)** $\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p_x\rangle$ and **b)** $\frac{d}{dt}\langle p_x\rangle = -\langle\frac{\partial V}{\partial x}\rangle$.

**Proof (a):**

$$\langle x\rangle = \int \psi^* \hat{x}\psi \; dx$$

$$\frac{d}{dt}\langle x\rangle = \frac{d}{dt}\int \psi^* \hat{x}\psi \ dx$$

$$= \int x(\psi \frac{\partial \psi^*}{\partial t} + \psi^* \frac{\partial \psi}{\partial t}) \ d\tau \qquad \text{……………… (a)}$$

The T.D.S.E. given by; $i\hbar\frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2\psi + V(r)\psi$ , So, divided by $i\hbar$ yields;

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\nabla^2\psi + \frac{V(r)\psi}{i\hbar} \qquad \text{……………... (b)}$$

The complex conjugate of (a) leads to;

$$\frac{\partial \psi^*}{\partial t} = \frac{-i\hbar}{2m}\nabla^2\psi^* - \frac{V(r)\psi^*}{i\hbar} \qquad \text{……………… (c)}$$

Substitute of equations (b and c) in (a) yields;

$$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\int (\psi^* x\nabla^2\psi - \psi \ x\nabla^2\psi^*) \ d\tau \qquad \text{…. …...…….. (d)}$$

Using Greens Theorem;

$$\int (\psi^*\nabla^2 x\psi - x\psi\nabla^2\psi^*) \ d\tau = \int (\psi^*\nabla x\psi - x\psi\nabla\psi^*)\cdot ds = 0$$

The boundary condition imposed on $\psi$ make the surface integral equal to zero. Where, the probability of finding the particle outside the volume is equal to zero i.e. the wave function $\psi$ is equal to zero on the surface.

$$\therefore \int (\psi^*\nabla^2 x\psi \ d\tau = \int x\psi\nabla^2\psi^* d\tau$$

Therefore, equation (d) becomes;

$$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\int (\psi^* x\nabla^2\psi - \psi^*\nabla^2 x\psi) \ d\tau \qquad \text{……………… (e)}$$

Since; $\nabla^2 x\psi = \nabla\cdot\nabla x \ \psi = x\nabla^2\psi + \nabla\psi + \nabla\psi$

$$\therefore \ \nabla^2 x\psi = x\nabla^2\psi + 2\frac{\partial}{\partial x}\psi \qquad \text{……………. (f)}$$

Substitute of equation (f) in (e) we get;

$$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\int (\psi^* x\nabla^2\psi - \psi^* x\nabla^2\psi - 2\psi^*\frac{\partial \psi}{\partial x}) \ d\tau$$

$$= \frac{-i\hbar}{m} \int \psi^* \frac{\partial \psi}{\partial x} d\tau$$

$$= \frac{1}{m} \int \psi^* (-i\hbar \frac{\partial}{\partial x}) \psi \; d\tau$$

$$= \frac{1}{m} \int \psi^* \hat{p}_x \psi \, d\tau$$

$$\therefore \quad \frac{d}{dt}\langle x \rangle = \frac{\langle p_x \rangle}{m}$$

**Proof (b):**

$$\langle p_x \rangle = \int \psi^* (-i\hbar \frac{\partial}{\partial x}) \; \psi \; d\tau$$

$$\frac{d}{dt}\langle p_x \rangle = -i\hbar \frac{d}{dt} \int \psi^* \frac{\partial \psi}{\partial x} d\tau$$

$$\frac{d}{dt}\langle p_x \rangle = i\hbar \int (\psi^* \frac{\partial}{\partial x} \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \frac{\partial \psi}{\partial x}) \; d\tau \qquad \ldots\ldots\ldots\ldots\ldots\ldots (a)$$

Regarding the T.D.S.E.: $i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi + V(r)\psi$ , and dividing by: $i\hbar$ yield;

$$\frac{\partial \psi}{\partial t} = \frac{-\hbar}{2mi} \nabla^2 \psi + \frac{V(r)\psi}{i\hbar} \qquad \ldots\ldots\ldots\ldots\ldots (b)$$

The complex conjugate leads to;

$$\frac{\partial \psi^*}{\partial t} = \frac{\hbar}{2mi} \nabla^2 \psi^* - \frac{V(r)\psi^*}{i\hbar} \qquad \ldots\ldots\ldots\ldots\ldots\ldots (c)$$

The substitution of (b) and (c) in (a) leads to;

$$\frac{d}{dt}\langle p_x \rangle = -i\hbar \int [\psi^* \frac{\partial}{\partial x} (\frac{-\hbar}{2mi} \nabla^2 \psi + \frac{V}{i\hbar} \psi) + (\frac{\hbar}{2mi} \nabla^2 \psi^* - \frac{V}{i\hbar} \psi^*) \frac{\partial \psi}{\partial x}] d\tau$$

$$\frac{d}{dt}\langle p_x \rangle = \int [\frac{\hbar^2}{2m} \psi^* \nabla^2 \frac{\partial \psi}{\partial x} - \psi^* \frac{\partial}{\partial x} V \psi - \frac{\hbar^2}{2m} \nabla^2 \psi^* \frac{\partial \psi}{\partial x} + V \psi^* \frac{\partial \psi}{\partial x}] d\tau$$

$$\frac{d}{dt}\langle p_x \rangle = -\int (\psi^* \frac{\partial}{\partial x} V \psi - V \psi^* \frac{\partial \psi}{\partial x}) \; d\tau - \frac{\hbar^2}{2m} \int [\frac{\partial \psi}{\partial x} \nabla^2 \psi^* - \psi^* \nabla^2 (\frac{\partial \psi}{\partial x})] d\tau$$

Apply Greens theorem on the second term we get;

$$\int [\frac{\partial \psi}{\partial x}\nabla^2 \psi^* - \psi^* \nabla^2 \frac{\partial \psi}{\partial x}] d\tau = \int [\frac{\partial \psi}{\partial x}\nabla \psi^* - \psi^* \nabla \frac{\partial \psi}{\partial x}] \cdot ds = 0$$

However, the integration of the first term is;

$$= -\int (\psi^* (V \frac{\partial \psi}{\partial x} + \psi \frac{\partial V}{\partial x}) - V \psi^* \frac{\partial \psi}{\partial x} \;\; d\tau$$

$$\frac{d}{dt}\langle p_x \rangle = -\int \psi^* \frac{\partial V}{\partial x} \psi \;\, d\tau$$

$$\frac{d}{dt}\langle p_x \rangle = -\langle \frac{\partial V}{\partial x} \rangle$$