For $\hat{A}$ to be a Constant of motion

$$\boxed{[\hat{H}, \hat{A}] = 0}$$

The Ehrenfest Theorem:

In quantum mechanics the expectation value of observables behave in the same way as the observables themselves do in the classical mechanics.

This is also known as the Corresponding Principle.

Let us take a simple example of one dimensional dynamical system. The velocity is the time rate of change of the expectation value of the position i.e

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

The only quantity that changes in time is $\psi(x,t)$ and it is the variation that gives rise to variation in $\langle x\rangle$.

The one-dimensional Schrodinger equ.
is

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi$$

The values of $\frac{\partial \psi}{\partial t}$ and $\frac{\partial \psi^*}{\partial t}$ are obtained from the Schrodinger equation and we get

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

Integration by parts gives

$$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\left\{\left[\psi^* x \frac{\partial \psi}{\partial x}\right|_{-\infty}^{\infty} - \int\left(\frac{\partial \psi^*}{\partial x} x \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial \psi}{\partial x}\right)dx\right.$$
$$\left. - \frac{\partial \psi^*}{\partial x} x\psi\right|_{-\infty}^{\infty} + \int\left(\frac{\partial \psi^*}{\partial x} x \frac{\partial \psi}{\partial x} + \frac{\partial \psi^*}{\partial x}\psi\right)dx\Bigg]$$

Since $\psi, \frac{\partial \psi}{\partial x} \longrightarrow 0$

as $x \longrightarrow \pm\infty$

we have

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

(6a)

Again integrating by parts the first term, we get

$$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\left[|\psi^* \psi|_{-\infty}^{\infty} - \int \psi^* \frac{\partial \psi}{\partial x} dx - \int \psi^* \frac{\partial \psi}{\partial x} dx \right]$$

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

$$= \frac{1}{m} \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, dx$$

$$= \frac{1}{m} \int \psi^* \hat{P}_x \psi \, dx, \quad \hat{P}_x = -i\hbar \frac{\partial}{\partial x}$$

momentum operator

$$\boxed{\frac{d}{dt}\langle x\rangle = \frac{\langle \hat{P}_x \rangle}{m}}$$

The correspond to the classical equ:

$$\frac{dx}{dt} = \frac{P_x}{m} \quad \text{or} \quad P_x = m \frac{dx}{dt}$$

Similarly we can calculate the rate of change of $\langle P_x \rangle$ as:

$$\frac{d}{dt}\langle P_x \rangle = \frac{d}{dt}\langle P_x \rangle = -i\hbar \frac{d}{dt}\int \psi^* \frac{\partial \psi}{\partial x}\, dx$$

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

Using Schrodinger equation, we get

$$\frac{d}{dt}\langle P_x \rangle = -\frac{\hbar^2}{2m}\int \left(\frac{\partial^2 \psi^*}{\partial x^2}\frac{\partial \psi}{\partial x} - \psi^* \frac{\partial^3 \psi}{\partial x^3} \right) dx$$

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

$$= -\frac{\hbar^2}{2m}\int \left\{ \frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial x}\frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right) \right\} dx$$

$$- \int \psi^* \frac{\partial V}{\partial x}\psi\, dx$$

$$= -\frac{\hbar^2}{2m}\left| \frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x} - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right|_{-\infty}^{\infty} = 0$$

$$- \int \psi^* \frac{\partial V}{\partial x}\psi\, dx$$

(7a)

$$\frac{d}{dt}\langle P_x \rangle = -\int \psi^* \frac{\partial V}{\partial x}\psi \, dx$$

$$= -\left\langle \frac{\partial V}{\partial x} \right\rangle$$

$$\boxed{\frac{d}{dt}\langle P_x \rangle = \langle F_x \rangle}; \quad F_x = -\frac{\partial V}{\partial x}$$

which corresponds to Newtons 2nd law of motion

$$\boxed{\frac{dP_x}{dt} = F_x}$$

Time-Independent and Time-Dependent Schrodinger Wave Equation:

The general 1-dimensional Schrodinger wave equation for a particle in potential $V(x)$ is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + V(x)\Psi = i\hbar\frac{\partial \Psi}{\partial t}$$

where $\Psi = \Psi(x,t)$.

Now separating Ψ into space and time components

$$\Psi = \psi(x)\,\phi(t)$$

This gives

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi(x)\phi(t)=i\hbar\frac{\partial}{\partial t}\left[\psi(x)\phi(t)\right]$$

$$-\frac{\hbar^2}{2m}\phi(t)\frac{\partial^2\psi}{\partial x^2}+V(x)\psi(x)\phi(t)=i\hbar\,\psi(x)\frac{\partial\phi}{\partial t}$$

Dividing both sides by $\psi\phi$, we get

$$-\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)=\frac{i\hbar}{\phi(t)}\cdot\frac{\partial\phi(t)}{\partial t}=C$$

Time-dependent equ:- $\frac{i\hbar}{\phi(t)}\cdot\frac{\partial\phi}{\partial t}=C$

Time-independent Equ:-

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi}{\partial x^2}+V(x)=C$$

The value of C is obtained as follows:

$$i\hbar\frac{1}{\phi}\frac{\partial\phi}{\partial t}=C$$

$$\frac{1}{\phi}\partial\phi=\frac{C}{i\hbar}\partial t$$

Integration gives.

$$\ln\phi(t)=\frac{C}{i\hbar}t+\text{Const}$$

Now suppose that the initial conditions are such that

$$\text{Const} = \text{zero}$$

$$\Rightarrow \quad \ln \phi(t) = -i \frac{c}{\hbar} t$$

$$\phi(t) = \exp\left(-i \frac{c}{\hbar} t\right)$$

Comparing this with a general Complex wavefunction

$$\phi(t) = \exp(-i\omega t)$$

$$\Rightarrow \quad \frac{c}{\hbar} = \omega$$

$$\boxed{c = \hbar\omega = E}$$

$\Rightarrow$ The time independent equation can be written as

$$-\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{\partial^2 \psi}{\partial x^2} + V(x) = E$$

or

$$\boxed{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + (V(x) - E)\psi(x) = 0}$$

and time-dependent will be in this form.

$$\boxed{i\hbar \frac{\partial \phi}{\partial t} = E\phi}$$

Examples: 3.5,
Solved Problem: 3.3, 3.6, 3.7, 3.8, 3.9, 3.10
Exercise: 3.26