

Expectation Value and Uncertainty;

Consider a particle with state vector $|\Psi\rangle$. The expectation value (or mean value) of an observable that is represented by the Hermitian operator Ω is:

$$\langle \Omega \rangle = \sum_{\omega} P(\omega) \omega \quad \text{where} \quad \Omega |\omega\rangle = \omega |\omega\rangle$$

$$\begin{aligned} P(\omega) &= |\langle \omega | \Psi \rangle|^2 \Rightarrow \langle \Omega \rangle = \sum_{\omega} \langle \Psi | \omega \rangle \langle \omega | \Psi \rangle \omega \\ &= \sum_{\omega} \langle \Psi | \omega \rangle \langle \omega | \Omega | \Psi \rangle = \left(\sum_{\omega} |\omega\rangle \langle \omega| \right) \Omega | \Psi \rangle = \\ &\langle \Psi | \Omega | \Psi \rangle \end{aligned}$$

Measuring the observable with an ensemble of N particles, prepared in the same state $|\Psi\rangle$, or measuring it N times with a single particle in the same state $|\Psi\rangle$, yields $\langle \Omega \rangle$ (for large N).

Uncertainty, or standard deviation, in an observable that is represented by the Hermitian operator is defined as:

$$\Delta \Omega = \left[\langle \Psi | (\Omega - \langle \Omega \rangle)^2 | \Psi \rangle \right]^{\frac{1}{2}} = \left[\langle \Psi | \Omega^2 | \Psi \rangle - \langle \Psi | \Omega | \Psi \rangle^2 \right]^{\frac{1}{2}}$$

If $|\Psi\rangle$ is an eigenvector of Ω , then:

$$\Omega |\Psi\rangle = \omega |\Psi\rangle \Rightarrow \langle \Psi | \Omega^2 | \Psi \rangle = \omega^2 \langle \Psi | \Psi \rangle = \omega^2$$

$$\langle \Psi | \Omega | \Psi \rangle^2 = \omega^2 \langle \Psi | \Psi \rangle = \omega^2$$

Thus:

$$\Delta \Omega = 0$$

Density Matrix:

For a particle in state $|\Psi\rangle$ (pure state), the density matrix ρ is defined as the operator:

$$\rho = |\Psi\rangle \langle \Psi|$$

It has the following properties:

$$\rho^\dagger = \rho \quad \text{Tr} \rho = 1 \quad \rho^2 = \rho$$

Now:

$$\text{Tr}(\Omega \rho) = \sum_i \langle i | \Omega | \psi \rangle \langle \psi | i \rangle$$

Where $|i\rangle$ form an orthonormal basis. If we choose the basis consisting of eigenvectors of Ω :

$$\begin{aligned} \text{Tr}(\Omega \rho) &= \sum_{\omega} \langle \omega | \Omega | \psi \rangle \langle \psi | \omega \rangle = \sum_{\omega} \omega |\langle \omega | \psi \rangle|^2 \\ &= \langle \Omega \rangle \end{aligned}$$

Density matrix contains all of the statistical information about the state $|\psi\rangle$.

The Schrodinger Equation and Time Evolution:

The Schrodinger equation is:

$$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle$$

If H is time-independent, then we have:

$$|\psi(t)\rangle = e^{-\frac{iHt}{\hbar}} |\psi(0)\rangle$$

where $|\Psi(0)\rangle$ is the state vector at the initial time $t=0$. Therefore if we know $|\Psi(0)\rangle$, we will know $|\Psi(t)\rangle$ for any t .

The operator $e^{-\frac{iHt}{\hbar}}$ is called the propagator and denoted by U .

Time evolution can be most conveniently described in the basis consisting of eigenvectors of the Hamiltonian H :

$$H|E\rangle = E|E\rangle$$

$$|\Psi(0)\rangle = \sum_E a_{(0)} |E\rangle$$

$$|\Psi(t)\rangle = e^{-\frac{iHt}{\hbar}} |\Psi(0)\rangle = e^{-\frac{iHt}{\hbar}} \sum_E a_{(0)} |E\rangle = \sum_E a_{(0)} e^{-\frac{iEt}{\hbar}} |E\rangle = \sum_E a_{(0)} e^{-\frac{iEt}{\hbar}} |E\rangle$$

Once we know $a_{(0)}$, then we will know $|\Psi(t)\rangle$.

This is why finding the eigenvalues and

eigenvectors of the Hamiltonian are so useful.

The probability to find value E_1 for the energy

is:

$$P(E_1) = |\langle E_1 | \Psi \rangle|^2 = \left| \langle E_1 | \sum_E a_E(t) e^{-\frac{iEt}{\hbar}} | E \rangle \right|^2$$

$$= |a_{E_1}(t)|^2$$

This implies that $P(E_1)$ is time-independent.

If the initial state is one of the eigenvectors of the Hamiltonian:

$$|\Psi(0)\rangle = |E_1\rangle$$

we have:

$$|\Psi(t)\rangle = e^{-\frac{iHt}{\hbar}} |E_1\rangle = e^{-\frac{iE_1 t}{\hbar}} |E_1\rangle$$

But this is just a pure phase. Therefore the system will always remain in the same state.