Quantum Mechanics - Lecture 6

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Uncertainty Relations

- The uncertainty (standard deviation) between the product of two operators can be derived as

$$\Delta A\ \Delta B\ \geq \frac{1}{2}\left[\hat{A},\hat{B}\right],\quad \text{(generalized uncertainty principle)}$$

The proof is given at:
Griffiths (second edition): Section 3.5, page 122
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$$\Delta y \, \Delta \mathrm{p_y} \geq \frac{1}{2}\left[\hat{y}, \hat{p}_y\right] \geq \frac{1}{2}\hbar$$

$$\Delta z \, \Delta \mathrm{p_z} \geq \frac{1}{2}[\hat{z}, \hat{p}_z] \geq \frac{1}{2}\hbar$$

- For every pair of observables whose operators do not commute (incompatible observables) there is an uncertainty relation. For example,

$$\left[\hat{\mathrm{L}}_{\mathrm{x}}, \hat{\mathrm{L}}_{\mathrm{y}}\right] = \mathrm{i}\hbar\, L_z \;\Rightarrow\; \Delta L_x\, \Delta L_{\mathrm{y}} \geq \frac{1}{2}\, \hbar < \hat{L}_z >$$ (orbital angular momentum uncertainty relations)

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\- Now lets us assume that the particle in the *s* state. Then, $< \hat{L}_z > = 0$. This implies that we can measure both L_x and L_y to the same accuracy. And this is because both L_x and L_y have the same eigen state, *s* state.

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- Every pair of compatible observables (because they can have the same eigen function), there is no uncertainty relation. And, we can measure them to the same accuracy.

For example: energy and momentum, different components of position and momentum, etc.

Energy and Time Uncertainty Relation

$$\Delta E \, \Delta t \geq \frac{1}{2} \hbar$$

"→ this is not derived from the general uncertainty relation as time is not a dynamical variable". Time is an independent variable, and dynamical variables such as position and momentum can be a function of time.

"→ Δt is the time interval between the measurements"

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- The energy-time uncertainty relation is useful in studying the decay process. In this case, Δt and ΔE represents the mean life time and the energy of the excited state, respectively.

Time-Independent Schrodinger equation

“stationary states”

- We know the time-dependent Schrodinger equation is

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(\mathrm{x},\mathrm{t}) \quad \text{Eq.(1)}$$

→ Wave function is time-dependent
→ Potential is time-independent

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- Now, lets separate the time-dependent wave function as

$$\Psi(x,t) = \psi(x)\phi(t) \qquad \text{Eq.(2)}$$

- From Eq.(2) we can write

$$\frac{\partial \Psi(x,t)}{\partial t} = \psi(x)\frac{d\phi(t)}{dt} \quad \text{and} \quad \frac{\partial^2 \Psi(x,t)}{\partial x^2} = \phi(t)\frac{d^2\psi(x)}{dx^2} \qquad \text{Eq.(3)}$$

- Using Eq.(3) in Eq.(1) and dividing by $\psi(x)\phi(t)$, we get

$$\mathrm{i}\hbar\frac{1}{\phi}\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V$$

- This we can also write

$$\mathrm{i}\hbar\frac{1}{\phi}\frac{d\phi}{dt} = E \qquad \text{and} \qquad -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E \qquad \text{(E is a constant)}$$

$$\Rightarrow \frac{d\phi}{dt} = -\frac{iE}{\hbar}\phi \qquad \text{and} \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

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  K. E. + P. E. = H (Hamiltonian)

- Therefore, we can write the time independent Schrodinger equation as $H\psi(x) = E\,\psi(x)$

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the solution can be obtained as

$$\phi(\mathrm{t}) = \mathrm{e}^{-\frac{iEt}{\hbar}}$$

→ represents the time-dependent part of the wave function

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- Therefore, the actual time dependent wave function is

$$\Psi(x,t) = \psi(x)\, e^{-\frac{iEt}{\hbar}}$$

"this is called the stationary state solution of the time-independent Schrodinger equation"

→ if potential is time independent, the time evolution of a wave function a simply the multiplication of $\psi(x)$ and a factor $e^{-\frac{iEt}{\hbar}}$

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- The probability density

$$|\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t) = \left(\psi(x)\, e^{-\frac{iEt}{\hbar}}\right)^* \left(\psi(x)\, e^{-\frac{iEt}{\hbar}}\right) = \psi^*(x)\psi(x) = |\psi(x)|^2$$

→ "probability density is independent of time"

- In the case of infinite set of solution $\psi_1(x), \psi_2(x), \psi_3(x), \ldots\ldots$ associated with energy $\mathrm{E}_1, \mathrm{E}_2, \mathrm{E}_3, \ldots\ldots$, respectively. The total wave function

$$\psi(x) = c_1\psi_1(x) + c_2\psi_2(x) + c_3\psi_3(x) + \ \ldots\ldots = \ \sum_{n=1}^{\infty} c_n\psi_n(x)$$

where, $c_n \ = \ \int \psi_n^*(x)\psi(x)dx$

- Now, the time dependent wave function is

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)\ e^{-\frac{iE_n t}{\hbar}}$$

→ $\Psi(x,t)$ here is NOT stationary in general as different $\psi's$ has different energy.

Continuity Equation

"conservation of probability"

- Consider the time-dependent Schrodinger equation in three dimension

$$i\hbar\frac{\partial\Psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(r,t) + V(r,t)\Psi(r,t) \qquad \text{Eq.(1)}$$

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- Taking the complex conjugate on both sides

$$-i\hbar \frac{\partial \Psi^*(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi^*(r,t) + V(r,t)\Psi^*(r,t) \qquad \text{Eq.(2)}$$

- Using $\Psi^*(r,t) \times \text{Eq.}(1) - \Psi(r,t) \times \text{Eq.}(2)$, we get

$$i\hbar\, \Psi^*(r,t)\frac{\partial \Psi(r,t)}{\partial t} + i\hbar\, \Psi(r,t)\frac{\partial \Psi^*(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\Psi^*(r,t)\,\nabla^2\Psi(r,t) + \frac{\hbar^2}{2m}\Psi(r,t)\,\nabla^2\Psi^*(r,t)$$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}\left(\Psi^*(r,t)\Psi(r,t)\right) = -\frac{\hbar^2}{2m}\left[\Psi^*(r,t)\,\nabla^2\Psi(r,t) - \Psi(r,t)\,\nabla^2\Psi^*(r,t)\right]$$

Using the relation $f_1\nabla^2 f_2 - f_2\nabla^2 f_1 = \nabla\cdot(f_1\nabla f_2 - f_2\nabla f_1)$

$$\Rightarrow \frac{\partial}{\partial t}\left(\Psi^*(r,t)\Psi(r,t)\right) = \frac{i\,\hbar}{2m}\vec{\nabla}\cdot\left[\Psi^*(r,t)\,\nabla\ \ \Psi(r,t) - \Psi(r,t)\,\nabla\ \ \Psi^*(r,t)\right]$$

We can write this equation in the form

$$\frac{\partial\rho(r,t)}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0 \quad \text{(the continuity equation)}$$

Where: $\rho(r,t) = \Psi^*(r,t)\Psi(r,t) \rightarrow$ called the probability density

$$\vec{J}(r,t) = \frac{i\,\hbar}{2m}\left[\Psi(r,t)\quad \nabla\Psi^*(r,t)\ - \ \Psi^*(r,t)\quad \nabla\Psi(r,t)\right]$$ $\rightarrow$ called the probability current density

Physical Interpretation:

Integrating the above continuity equation over a volume *V* bounded by a surface *S*, we get

$$\int_V \left(\frac{\partial \rho(r,t)}{\partial t} + \vec{\nabla}\cdot\vec{J}\right) dV = 0 \Rightarrow \int_V \frac{\partial \rho(r,t)}{\partial t}\, dV = -\int_V (\vec{\nabla}\cdot\vec{J}) dV$$

$$\Rightarrow \oint_S \vec{J}\cdot d\vec{S} = -\frac{d}{dt}\int_V \rho(r,t) dV$$

→ flow of probability out through the surface is equal to the decrease in the probability of finding the particle in the volume.

→ total probability must be conserved

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Analogy with other continuity equations:

$$\nabla\cdot J + \frac{\partial \rho}{\partial t} = 0$$

(Electromagnetism)

$$\nabla\cdot(\rho v) + \frac{\partial \rho}{\partial t} = 0$$

(Fluid Dynamics)

$$\nabla\cdot E + \frac{\partial u}{\partial t} = 0$$

(Heat and Energy)

Example Problem 3: Prove the commutation relation

$$\left[\hat{L}_x\,,\hat{L}_y\right] = i\hbar\,\hat{L}_z$$

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$$[\hat{L}_x , \hat{L}_y] = i\hbar \, \hat{L}_z$$

Solution: We know that $\vec{L} = \vec{r} \times \vec{p}$. Using this we can write

$$\hat{L}_x = -i\hbar \left(\hat{y} \frac{\partial}{\partial z} - \hat{z} \frac{\partial}{\partial y} \right),$$

$$\hat{L}_y = -i\hbar \left(\hat{z} \frac{\partial}{\partial x} - \hat{x} \frac{\partial}{\partial z} \right),$$

$$\hat{L}_z = -i\hbar \left(\hat{x} \frac{\partial}{\partial y} - \hat{y} \frac{\partial}{\partial x} \right)$$

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$$\hat{L}_z = -i\hbar\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)$$

$$\left[\hat{L}_x\,,\hat{L}_y\right] = \hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x$$

$$= -\hbar^2\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)\left(\hat{z}\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right) + \hbar^2\left(\hat{z}\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right) - i\hbar\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)$$

$$= \hbar^2\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right) = -i^2\,\hbar^2\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)$$

$$= i\hbar\left[-i\hbar\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)\right]$$

$$= i\hbar\,\hat{L}_z$$

Similarly, we can prove that

$$[\hat{L}_y, \hat{L}_z] = i\hbar\, \hat{L}_x$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar\, \hat{L}_y$$

$$[\hat{L}_x, \hat{L}_x] = 0$$

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