Lecture Four

4-1 Properties of the wave Function:

To be an acceptable solution, Ψ *and* $\frac{\partial\Psi}{\partial x}$ must be satisfying the following the restrictions for all values of x:

1- Ψ and $\frac{\partial\Psi}{\partial x}$ must be finite.
2- Ψ and $\frac{\partial\Psi}{\partial x}$ must be continuous.

4-2 Operator:

An operator, O (say), is a mathematical entity which transforms one function into another: i.e.,

$$O\,(f(x)) \rightarrow g(x). \qquad 4\text{-}1$$

For instance, x is an operator, since x f (x) is a different function to f (x), and is Fully specified once f (x) is given. Furthermore, d/dx is also an operator, since $\frac{df(x)}{dx}$ is a different function to f(x), and is fully specified once f (x) is given.

Now,

$$x\frac{d}{dx} \neq \frac{d}{dx}(xf) \qquad 4-2$$

This can also be written

$$x\frac{d}{dx} \neq \frac{d}{dx}\,x \qquad 4-3$$

Where the operators are assumed to act on everything to their right, and a final

f (x) is understood [where f (x) is a general function]. The above expression illustrates an important point: i.e., in general, operators do not commute. Of course, some operators do commute: e.g.,

$$x\, x^2 = x^2\, x$$

Finally, an operator, O, is termed ***linear*** if

$$O\,(cf\,(x) = c\,O\,\big(f(x)\big) \qquad 4-4$$

Where f (x) is a general function, and c a general complex number. All of the operators employed in quantum mechanics are ***linear***.

Now, from the following Eqs:

$$\langle x\rangle = \int_{-\infty}^{\infty} \Psi^*\, x\, \Psi\, dx, \qquad 4-5$$

$$\langle p\rangle = \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar\frac{\partial}{\partial x}\right)\Psi\, dx \qquad 4-6$$

These expressions suggest a number of things. First, classical dynamical variables, such as x and p, are represented in quantum mechanics by linear operators which act on the wave-function. Second, displacement is represented by the algebraic operator x, and momentum by the differential operator $-i\hbar\frac{\partial}{\partial x}$: i.e.,

$$p = -i\hbar\frac{\partial}{\partial x} \qquad 4-7$$

Finally, the ***<u>Expectation value</u>*** of some dynamical variable represented by the operator O(x) is simply

$$\langle O\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\, O(x)\, \psi(x,t)\, dx. \qquad 4-8$$

Clearly, if an operator is to represent a dynamical variable which has physical significance then its expectation value must be real. In other words, if the Operator O represents a physical variable then we require that < O> = <O>*; or

$$\int_{-\infty}^{\infty} \psi^* (O\,\psi)\, dx = \int_{-\infty}^{\infty} (O\,\psi)^*\, \psi\, dx,$$

where O^* is the complex conjugate of O. An operator which satisfies the above

Constraint is called a ***Hermitian operator***. It is easily demonstrated that x and

p are both Hermitian. The Hermitian conjugate, $O^\dagger$, of a general operator, O, is defined as follows:

$$\int_{-\infty}^{\infty} \psi^* (O\,\psi)\, dx = \int_{-\infty}^{\infty} (O^\dagger\,\psi)^*\, \psi\, dx.$$

The Hermitian conjugate of an Hermitian operator is obviously the same as the operator itself: *i.e.*, $p^\dagger = p$. For a non-Hermitian operator, O (say), it is easily demonstrated that $(O^\dagger)^\dagger = O$, and that the operator $O + O^\dagger$ is Hermitian. Finally, if A and B are two operators, then $(A\,B)^\dagger = B^\dagger A^\dagger$.

The properties of Hermitian operator are:

1- The eigenvalues of a Hermitian operator are all real. (**Please Prof that**).
2- The Eigen functions of a Hermitian operator are orthogonal if the corresponding Eigen values are unequal. (**Prove that**).

Where the orthonormal is: $\int_{-\infty}^{\infty} \Psi^*\, \Psi\, dx = 0$

4-3 Commute operator and commutation relation:

The commutation relations of two operators are:

$$[\hat{O},\hat{R}]\Psi = \hat{O}\hat{R}\Psi - \hat{R}\hat{O}\Psi$$

If $[\hat{O},\hat{R}] = 0$, this mean that the operator O is commute with the operator R.

Example: - prove that $[\hat{x},\hat{p}] = -i\hbar$

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

$$= -i\hbar\left(x\frac{\partial\Psi}{\partial x} - \Psi - x\frac{\partial\Psi}{\partial x}\right) = +i\hbar\Psi \neq 0 \text{ they do not commute}$$

Prove also: $[\hat{y},\hat{p}_y] = [\hat{z},\hat{p}_z] = i\hbar$

But $[\hat{x},\hat{p}_y] = 0$ *this mean that operator* $\hat{x}$ *are commute with* p_y

$$[\hat{r}_i,\hat{p}_j] = i\hbar\delta_{ij}$$

Where $\delta_{ij} = 0 \ \ or\ 1$

Let's now briefly go over how to perform algebraic manipulations using operators and commutators. These are straightforward to prove

1. $[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$
2. $[\hat{A},\hat{A}] = -[\hat{A},\hat{A}] = 0$
3. $[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$
4. $[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]$
5. $[\hat{A},[\hat{B},\hat{C}]] + [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]] = 0$ (Jacobi Identity)
6. $[\hat{A},\hat{B}]^\dagger = [\hat{A}^\dagger,\hat{B}^\dagger]$

Example .1 Write down the velocity operator $\hat{v}$, and its expectation value.

Solution We have $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ and $p = mv$. Thus we *define* the velocity operator

$$\hat{v} \equiv \frac{\hat{p}}{m}$$

Thus

$$\hat{v} = -\frac{i\hbar}{m}\frac{\partial}{\partial x}$$

The expectation value would be

$$\begin{aligned}\langle v \rangle &= \int \Psi^* \left(-\frac{i\hbar}{m}\frac{\partial}{\partial x}\right) \Psi \, dx \\ &= -\frac{i\hbar}{m}\int \Psi^* \frac{\partial \Psi}{\partial x} dx\end{aligned}$$

linear momentum operator

Classical Mechanics $\Rightarrow \frac{dx}{dt} = \frac{P_x}{m}$

Quantum Mechanics $\Rightarrow \frac{d}{dt}\langle x\rangle = \frac{\langle P_x\rangle}{m}$

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\int \psi^* \hat{P}_x \psi \, dx$$

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

$$= \int x \frac{\partial}{\partial t}(\psi^* \psi)\, dx = \int x \frac{\partial}{\partial t} P(x,t)\, dx$$

From the Continuity eq. $\frac{\partial P}{\partial t} + \frac{\partial}{\partial x} S_x = 0$

$$\therefore \frac{d}{dt}\langle x\rangle = -\int x \frac{\partial S_x}{\partial x}\, dx$$

$$= -\left\{ \int_{-\infty}^{\infty} \frac{d}{dx}[x S_x]\, dx - \int_{-\infty}^{\infty} S_x \, dx \right\}$$

$$= -\underbrace{[x S_x]_{-\infty}^{\infty}}_{\text{zero}} + \int_{-\infty}^{\infty} S_x \, dx = \int_{-\infty}^{\infty} S_x \, dx$$

$$= \int_{-\infty}^{\infty} \frac{\hbar}{2mi} \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right) dx$$

$$\int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \psi \, dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial x} (\psi^* \psi) \, dx - \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

$$= \underbrace{(\psi^* \psi) \Big|_{-\infty}^{\infty}}_{0} - \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

$$\therefore \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \psi \, dx = \int_{-\infty}^{\infty} - \psi^* \frac{\partial \psi}{\partial x} dx$$

$$\Rightarrow \frac{d}{dt} \langle x \rangle = \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{mi} \frac{\partial}{\partial x} \psi \, dx$$

$$\frac{\langle P_x \rangle}{m} = \frac{1}{m} \int_{-\infty}^{\infty} \psi^* \hat{P}_x \psi \, dx$$

$$\therefore \int \psi^* \frac{\hbar}{i} \frac{\partial}{\partial x} \psi \, dx = \int \psi^* \hat{P}_x \psi \, dx$$

$$\boxed{\begin{aligned} \therefore \hat{P}_x &= -i\hbar \frac{\partial}{\partial x} \\ \hat{\vec{P}} &= -i\hbar \vec{\nabla} \end{aligned}}$$

momentum operator

The Hamiltonian operator

The total energy of a particle.

$$E = \frac{P^2}{2m} + V$$

$$P \longrightarrow \hat{P} = -i\hbar \frac{\partial}{\partial x}$$

$$V \longrightarrow \hat{V}$$

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

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

Hamiltonian operator in one-dimension

Eigen value and eigen function

Denote by $\hat{Q}$, the operator associated with the observal q, then a measurment of q gives a result which is one of the values of the "eigen value" equation:

$$\hat{Q}\,\psi_n = q_n \psi_n$$

q_n is the eigen value

ψ_n is the eigen function

ex Sch. eq.

$$\hat{H}\psi_n = E_n\psi_n$$

This gives eigen values (energy levels) of a particle for some bound state system

$$E_1, E_2, E_3, \ldots$$

Degeneracy

If there are n linearly independent eigen ~~value~~ functions corresponding to the eigen value q, then, the eigen value is n-th order degenerate.

$$\left.\begin{aligned} \hat{Q}\psi_1 &= q\psi_1 \\ \hat{Q}\psi_2 &= q\psi_2 \\ &\vdots \\ \hat{Q}\psi_n &= q\psi_n \end{aligned}\right\} \text{degenerate states}$$

"وجود دوال موجية مختلفة تمثل حالات ديناميكية مختلفة لكنها تقابل نفس مستوى الطاقة n."

$$E_n = (n+1)\hbar\omega \quad , \quad E_{(n_x, n_y)} = (n_x + n_y + 1)\hbar\omega$$

n	n_x	n_y	$E(h\nu)$	
0	0	0	1	} one-form degenercy
1	1	0	2	} different state with the same energy
1	0	1	2	
2	2	0	3	} "3-form degenercy"
	1	1	3	
	0	2	3	

Also, the linear combination of degenerate state is an eigen value state with the same eigen value.

$$\Psi = \sum_n c_n \Psi_n$$

$$\hat{Q}\Psi = \sum_n c_n \hat{Q}\Psi_n = q \sum_n c_n \Psi_n = q\Psi$$

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Non-degenerate states / There is one ~~indepen~~ independent state associated with a given eigen value,

$$\hat{Q}\Psi_a = q_a \Psi_a$$

If another state, say ϕ, with the same eigenValue q_a then this State is not independent, but must be equal to the state Ψ_a multiplied by a multiplicative Constant such that

$$\phi = \alpha \Psi_a$$

$$\hat{Q}\phi = \alpha \hat{Q} \Psi_a = \alpha q_a \Psi_a = q_a \phi$$

*Problem 4-1 A particle of mass m is in the state

$$\Psi(x,t) = Ae^{-a[(mx^2/\hbar)+it]},$$

where A and a are positive real constants.

(a) Find A.

(b) For what potential energy function $V(x)$ does Ψ satisfy the Schrödinger equation?

(c) Calculate the expectation values of x, x^2, p, and p^2.

(d) Find σ_x and σ_p. Is their product consistent with the uncertainty principle?