University of Mosul
College of Science
Department of Physics
Fourth Class
Lecture 3

Quantum Mechanics

2023-2024

Lecture 3: Requirements of eigen function

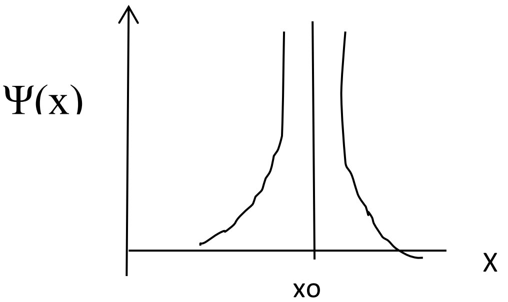
Preparation

Assist. prof. Alaa Abdul Hakeim

2.4 Requirements of eigen function

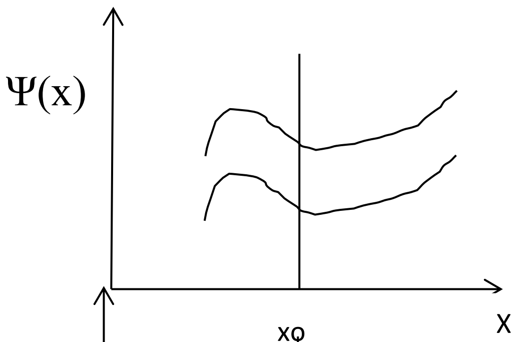
An eigen function Ψ(x) and its first derivative $\frac{\partial \Psi(x)}{\partial x}$ are required to have the following properties, to be acceptable solution for schrӧedinger equation :

1- Ψ(x) and $\frac{\partial \Psi(x)}{\partial x}$ must be finit.
2- Ψ(x) and $\frac{\partial \Psi(x)}{\partial x}$ must be single valued.
3- Ψ(x) and $\frac{\partial \Psi(x)}{\partial x}$ must be continuous.

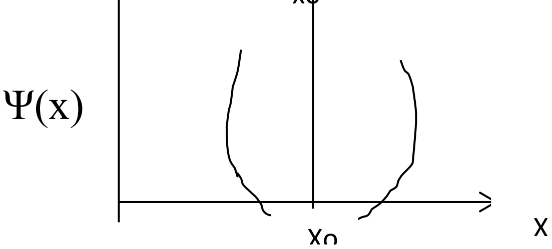


Not finit at Xo

finit does not be X at any point



not singled valued at Xo



Not continuous at Xo

These requirements are imposed in order to ensure that the eigen function be a mathematically well-behaved function so that measurable quantities which can be evaluated from the quantities which can be evaluated from the eigen function will also be well behaved.

<u>Problem 2.7</u>

Show that the operator $\hat{A} = \frac{\partial^2}{\partial x^2}$ has two possible eigen function

$U(x)=\sin kx$ and $U(x)=\cos kx$ and eigen value $(-k^2)$ for any k.but that if in addition the boundary condition U(0)=0 , U(L)=0 has to be satisfied ,than the eigen function are restricted to

$U_n=\sin\frac{n\,\pi x}{L}$, n=1,2,3,-------------

And eigen values are $a_n=-\frac{n^2\pi^2}{L^2}$, n=1,2,3,--------------

What are the eigen functions and eigen values for the boundary conditions that $\frac{\partial U}{\partial x}=0$ for x=0 and U=0 for x=L?

Solution:

$$\hat{A}U(x)=const.U(x)$$

$$\frac{\partial^2}{\partial x^2}sinkx=-k^2sinkx$$

Similarly

$$\frac{\partial^2}{\partial x^2}coskx=-k^2coskx$$

(a) The boundary condition U(0)=0 is satisfied by sinkx, but not by coskx to satisfy the condition U(L)=0, we must have sinkL=0

(kL=nπ =180,360,540,-------)

kL= nπ where n= 1,2,3,----------

hence $U_n=\sin\frac{n\,\pi x}{L}$ and $a_n=-\frac{n^2\pi^2}{L^2}$

(b) The condition $\frac{\partial U}{\partial x}=0$ when x=0 is satisfied by coskx, but not by sinkx

(because $\frac{\partial}{\partial x}coskx=-ksinkx=0\ for\ x=0$)

$$\frac{\partial}{\partial x}sinkx=kcoskx=1\neq 0\ for\ x=0$$

The condition U=0 for x=L requires

kL=$(n+\frac{1}{2})\pi$. Hence now

$$U_n=cos\frac{(n+\frac{1}{2})\pi}{L}x \quad , \qquad a_n=-\frac{(n+\frac{1}{2})^2}{L^2}\pi^2$$

2.5 A non-commutative properties of operators

If PQ = QP we say the two quantities P and Q commute with each other.

If PQ$\neq$ QP $\rightarrow$ PQ - QP$\neq$ 0

P and Q are not commute with each other in short notation we can put the relation

$[P, Q] \neq 0$ while $[\hat{A}, \hat{B}] = 0$

Means $\hat{A}$ *and* $\hat{B}$ commute with each other those relations called commutation relation.

If two operators commute with each other say, $[\hat{A}, \hat{B}] = 0$

This means $\hat{A}\hat{B} - \hat{B}\hat{A} = 0$

$\hat{A}\hat{B} = \hat{B}\hat{A}$ and this case

1- We can apply $\hat{A}\hat{B}$ *or* $\hat{B}\hat{A}$ on a function in any order.
2- A and B the dynamical variables belong to $\hat{A}$ *and* $\hat{B}$ do not obey the uncertainty principle, i.e. we can measure these dynamical variables exactly simultaneously.
3- $\hat{A}$ *and* $\hat{B}$ have the same eigen function and the advantage of this that we can evaluate the eigen function $\hat{A}$ as we know $\hat{B}$ e.f. when it is difficult to evaluate it for $\hat{A}$.

While if

$$[\hat{P}, \hat{Q}] \neq 0 \rightarrow \hat{P}\hat{Q} - \hat{Q}\hat{P} \neq 0 \rightarrow \hat{P}\hat{Q} \neq \hat{Q}\hat{P}$$

The two operator are not commute with each other , and we must apply them on a function in specified order and

1- We cannot measure the dynamically variables belonging to $\hat{P} and \hat{Q}$ exactly at the same time.
2- i.e. the two dynamical variables obey the uncertainty principle
3- $\hat{P} and \hat{Q}$ have different eigen function.

The operators involved in Q.M. do not all commute with each other. Thus when working with operators for dynamical variables in Q.M. it is essential that the order of the operation is properly specified.

Commutation laws of operators:

1- Addition is commutative

$$(\hat{A} + \hat{B})\Psi(x) = \hat{A}\Psi(x) + \hat{B}\Psi(x)$$

2- Multiplication, mostly, is not commutative

$\hat{A}\hat{B} \neq \hat{B}\hat{A}$ in special case $\hat{A}\hat{B} = \hat{B}\hat{A}$

3- $(\hat{A}\hat{B})\Psi(x) = \hat{A}(\hat{B}\,\Psi(x))$

Problem 2.8

Evaluate $\left[x, \frac{\partial}{\partial x}\right]$

Solution: $\left[x, \frac{\partial}{\partial x}\right] \ \Psi(x) = (x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x)\Psi(x)$

$=x\frac{\partial\Psi}{\partial x} - \Psi(x) - x\frac{\partial\Psi}{\partial x}$ =- $\Psi(x)$

$$\left[x, \frac{\partial}{\partial x}\right] = -1$$

Problem 2.9

Evaluation the following commutation relation.

$\left[\frac{\partial}{\partial x}, \frac{\partial^n}{\partial x^n}\right]$

Solution:

$\left[\frac{\partial}{\partial x}, \frac{\partial^n}{\partial x^n}\right] \Psi(\text{x})=(\frac{\partial}{\partial x}\frac{\partial^n}{\partial x^n} - \frac{\partial^n}{\partial x^n}\frac{\partial}{\partial x})\Psi(x)$

$=(\frac{\partial^{n+1}}{\partial x^{n+1}} - \frac{\partial^{n+1}}{\partial x^{n+1}})\Psi(x)$=0

$$\left[\frac{\partial}{\partial x}, \frac{\partial^n}{\partial x^n}\right] = 0$$

Problem 2.10

If three operators $\hat{A}, \hat{B}\ and \hat{C}$ are such that

$$\left[\hat{A}, \hat{B}\right] = 0\ , \ \left[\hat{A}, \hat{C}\right] \neq 0\ , \quad , \ \left[\hat{B}, \hat{C}\right] \neq 0$$

Show that

1- $\left[\hat{A}, \hat{B}\hat{C}\right] = \hat{B}\left[\hat{A}, \hat{C}\right]$
2- $\left[\hat{A}, \hat{A}\hat{B}\right] = 0$

3- $[\hat{A},[\hat{B},\hat{C}]] = [\hat{B},[\hat{A},\hat{C}]]$

Solution:

1. $[\hat{A},\hat{B}\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A}$

$[\hat{A},\hat{B}] = 0$ i.e. $\hat{A}\hat{B} = \hat{B}\hat{A}$

$[\hat{A},\hat{B}\hat{C}] = \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A}$

$= \hat{B}(\hat{A}\hat{C} - \hat{C}\hat{A})$

$= \hat{B}[\hat{A},\hat{C}]$

2. $[\hat{A},\hat{A}\hat{B}] = \hat{A}\hat{A}\hat{B} - \hat{A}\hat{B}\hat{A}$

$\hat{A}\hat{B} = \hat{B}\hat{A}$

$[\hat{A},\hat{A}\hat{B}] = \hat{A}\hat{A}\hat{B} - \hat{A}\hat{A}\hat{B} = 0$

3. H.W

Problem 2.11

Show that $[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$

Solution:

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = -(\hat{B}\hat{A} - \hat{A}\hat{B})$$
$$= -[\hat{B},\hat{A}]$$