Chapter 1

Tools of Quantum Mechanics

5. Commutator in Quantum Mechanics

Commutator: if $\hat{A}$ and $\hat{B}$ are two operators then the commutator $\left[\hat{A},\hat{B}\right]$ is defined as

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

Properties of Commutator:

- Antisymmetric $[\hat{A},\hat{B}]=-[\hat{B},\hat{A}]$
- Linearity $\left[\hat{A},\hat{B}+\hat{C}+\hat{D}\right]=\left[\hat{A},\hat{B}\right]+\left[\hat{A},\hat{C}\right]+\left[\hat{A},\hat{D}\right]$
- Distributivity: $\left[\hat{A}\hat{B},\hat{C}\right]=\left[\hat{A},\hat{C}\right]\hat{B}+\hat{A}\left[\hat{B},\hat{C}\right]$

  $\left[\hat{A},\hat{B}\hat{C}\right]=\left[\hat{A},\hat{B}\right]\hat{C}+\hat{B}\left[\hat{A},\hat{C}\right]$
- Jacobi Identity $\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]=0$
- Hermitian conjugate to commutator $\left([\hat{A},\hat{B}]\right)^{\dagger}=[\hat{B}^{\dagger},\hat{A}^{\dagger}]$
- $\left[\hat{A},a\right]=0$

- $\left[\hat{A},\hat{B}^n\right]=\sum_{j=0}^{n-1}\hat{B}^j\left[A,B\right]\hat{B}^{n-j-1}$

  $\left[\hat{A}^n,\hat{B}\right]=\sum_{j=0}^{n-1}\hat{A}^{n-j-1}\left[A,B\right]\hat{A}^j$

Commuting operators and Simultaneous Eigenfunctions

Consider two operators $\hat{A}$ and $\hat{B}$ which represent observables and are and are therefore Hermitian. If there is a $|\psi\rangle$ such that $\hat{A}|\psi\rangle=a|\psi\rangle$ and $\hat{B}|\psi\rangle=b|\psi\rangle$, then $|\psi\rangle$ is a simultaneous eigenfunction of $\hat{A}$ and $\hat{B}$, belonging to eigenvalues a and b, respectively.

Hence $\hat{B}\hat{A}|\psi\rangle=\hat{B}\left(a|\psi\rangle\right)=a\hat{B}|\psi\rangle=ab|\psi\rangle$ and $\hat{A}\hat{B}|\psi\rangle=\hat{A}\left(b|\psi\rangle\right)=b\hat{A}|\psi\rangle=ba|\psi\rangle$

$\Rightarrow\left(\hat{A}\hat{B}-\hat{B}\hat{A}\right)|\psi\rangle=0$ Thus $|\psi\rangle$ is also an eigenfunction of $\left[\hat{A},\hat{B}\right]$, belonging to the eigenvalue zero.

If $\hat{A}$ and $\hat{B}$ commute, then $\left[\hat{A},\hat{B}\right]|\psi\rangle=0$ holds for any $|\psi\rangle$.

Now we can show that the eigenfunctions of two commuting operators can always be constructed in such a way that they are simultaneous eigenfunctions.

Proof: Suppose $|\psi\rangle$ is an eigenfunction of $\hat{A}$, so

$\hat{A}|\psi\rangle=a|\psi\rangle$ and suppose $\hat{A}$ and $\hat{B}$ commute.

Then $\hat{B}\hat{A}|\psi\rangle=\hat{A}\hat{B}|\psi\rangle=\hat{B}a|\psi\rangle=a\hat{B}|\psi\rangle$

or $\hat{A}\left(\hat{B}|\psi\rangle\right)=a\left(\hat{B}|\psi\rangle\right)$

Thus, if we assume $\hat{B}|\psi\rangle\neq 0$, the function $\hat{B}|\psi\rangle$ is an eigenfunction of $\hat{A}$ belonging to the same eigenvalue, a. Two cases to consider:

(i) Nondegenerate case: If there is only one state $|\psi\rangle$ corresponding to the eigenvalue a, then $\hat{B}|\psi\rangle$ can differ from $|\psi\rangle$ only by a constant factor, or $\hat{B}|\psi\rangle=b|\psi\rangle$.

Hence, in this case, $\left[\hat{A},\hat{B}\right]|\psi\rangle=0$ is both a necessary and sufficient condition for $|\psi\rangle$ to be a simultaneous eigenfunction of $\hat{A}$ and $\hat{B}$.

(ii) Degenerate Case: Suppose, for example, that there are two states corresponding to the eigenvalue a, $|\psi_1\rangle$ and $|\psi_2\rangle$. These must be linearly independent and may for convenience be assumed to be orthonormal. Any linear combination $|\psi\rangle=c_1|\psi_1\rangle+c_2|\psi_2\rangle$ is also an eigenfunction of $\hat{A}$ but need not be an eigenfunction of $\hat{B}$. However, we can try to determine a particular linear combination(s), which will be an eigenfunction of $\hat{B}$, such that

$$\hat{B}\left(c_1|\psi_1\rangle + c_2|\psi_2\rangle\right) = b\left(c_1|\psi_1\rangle + c_2|\psi_2\rangle\right)$$

Taking scalar products with $|\psi_1\rangle$ and $|\psi_2\rangle$, respectively, we obtain

$$\hat{B}_{11} = \langle\psi_1|\hat{B}|\psi_1\rangle, \hat{B}_{22} = \langle\psi_2|\hat{B}|\psi_2\rangle, \hat{B}_{12} = \langle\psi_1|\hat{B}|\psi_2\rangle, \hat{B}_{21} = \langle\psi_2|\hat{B}|\psi_1\rangle$$

$$c_1B_{11} + c_2B_{12} = bc_1 + c_2.0 \Rightarrow c_1B_{11} + c_2B_{12} = bc_1$$

$$c_1B_{21} + c_2B_{22} = c_1.0 + bc_2 \Rightarrow c_1B_{21} + c_2B_{22} = bc_2$$

$c_1\left(\hat{B}_{11} - b\right) + c_2\hat{B}_{12} = 0$ with, etc.

$$c_1\hat{B}_{21} + c_2\left(\hat{B}_{22} - b\right) = 0$$

Nontrivial solution exists if $\begin{vmatrix} \hat{B}_{11} - b & \hat{B}_{12} \\ B_{21} & \hat{B}_{22} - b \end{vmatrix} = 0$

If the two roots b_1 and b_2 of the secular equation are distinct, the corresponding eigenfunctions of $\hat{B}$ are linearly independent. Hence the degeneracy has been resolved via the commuting operator $\hat{B}$.

If the roots b_1 and b_2 are the same, then if $\hat{B}$ is Hermitian, $\hat{B}_{11} = \hat{B}_{22}$ and $\hat{B}_{12} = B_{21^*} = 0$ are necessary and sufficient conditions. Accordingly any c_1 and c_2 can be used; i.e., $|\psi_1\rangle$ and ψ_2 are simultaneous, degenerate eigenfunctions of $\hat{B}$ as well as $\hat{A}$.

The analysis can be generalized immediately to cases of N- fold degeneracy. If the secular equation in b has N distinct roots, the degeneracy is completely resolved.

If the roots are not all distinct, it may be possible to find a third operator $\hat{C}$ which commutes with $\hat{A}$ and $\hat{B}$ and which will further resolve the remaining degeneracy, and do on. Ultimately, an unambiguous description of the system can be obtained in terms of a complete set of commuting observables, the eigenvalues of which provide a unique, nondegenerate specification of each state.

Set of commuting observables

- If two operators A and B commute and if $|\psi\rangle$ is eigen vector of A, then $B|\psi\rangle$ is also an eigen vector of A, with the same eigen value.

- If two operators A and B commute and if $|\psi_1\rangle$ and $|\psi_2\rangle$ are two eigen vector of A with different eigen values then Matrix element $\langle\psi_1|B|\psi_2\rangle$ is zero.
- If two operators A and B commute one can construct an orthonormal basis of state space with eigen vectors common to A and B.

Functions of Operator

Function of linear operator $F(\hat{A})$ can be expand as polynomial of $\hat{A}$ as $F(\hat{A})=\sum_n a_n\hat{A}^n$

For example, $\exp(a\hat{A})=\sum_n \frac{a^n}{\lfloor n}\hat{A}^n$

If two operator $F(\hat{A})$ and $G(\hat{A})$ are function of operator $\hat{A}$ then commutator $\left[F(\hat{A}),G(\hat{A})\right]=0$

If commutator $\left[\hat{A},\hat{B}\right]=0$ then $\left[B,F(\hat{A})\right]=0$

$\left[F(A)\right]^\dagger=F^*(A^\dagger)$ for example, $\left[\exp(iaA)\right]^\dagger=\exp(-ia^*A^\dagger)$

$$\exp(\hat{A}).\exp(\hat{B})=\exp(\hat{A}+\hat{B}).\exp\frac{[A,B]}{2}$$

$$\exp(\hat{A})\hat{B}\exp(-\hat{A})=\hat{B}+\left[\hat{A},\hat{B}\right]+\frac{1}{\lfloor 2}\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]+\frac{1}{\lfloor 3}\left[\hat{A},\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]\right].....$$

Example: If momentum operator $\hat{P}_x$ is defined as $-i\hbar\frac{\partial}{\partial x}$ and position operator X is defined as $\hat{X}\psi(x)=x\psi(x)$

(a) Find the value of commutator $[\hat{X},\hat{P}_x]$

(b) Using the property of commutator find the value of $[\hat{X}^2,\hat{P}_x]$ and $[\hat{X},\hat{P}_x^2]$

(c) Using the property find the value of $\left[\hat{X}^2,\hat{P}_x^2\right]$

Solution: (a): $[\hat{X},\hat{P}_x]=(\hat{X}\hat{P}_x-\hat{P}_x\hat{X})$

Operator both side with ψ

$$\hat{X}\hat{P}_x\psi(x)-\hat{P}_x\hat{X}\psi(x)$$

$$\hat{X}(-i\hbar)\frac{\partial\psi(x)}{\partial x}-\hat{P}_x x\psi(x)$$

$$\hat{X}\left(-i\hbar\right)\frac{\partial\psi\left(x\right)}{\partial x}+i\hbar\frac{\partial}{\partial x}x\psi(x)$$

$$x\left(-i\hbar\right)\frac{\partial\psi\left(x\right)}{\partial x}+x\ i\hbar\frac{\partial\psi\left(x\right)}{\partial x}+i\hbar\frac{\partial x}{\partial x}\psi(x)=i\hbar\psi\left(x\right)$$

$$[\hat{X},\hat{P}_x]=i\hbar\psi(x) \qquad [\hat{X},\hat{P}_x]=i\hbar$$

(b) $$[\hat{X}^2,\hat{P}_x]=[\hat{X}\cdot\hat{X},\hat{P}_x]=\hat{X}[\hat{X},\hat{P}_x]+[\hat{X},\hat{P}_x]\hat{X}=\hat{X}i\hbar+i\hbar\hat{X}=2i\hbar\hat{X}$$

$$[\hat{X},\hat{P}_x^2]=[\hat{X},\hat{P}_x\cdot\hat{P}_x]$$

$$\hat{P}_x[\hat{X},\ \hat{P}_x]+[\hat{X},\hat{P}_x]\hat{P}_x=\hat{P}_x i\hbar+i\hbar\hat{P}_x \qquad [\hat{X},\hat{P}_x^2]=2i\hbar\hat{P}_x$$

(c) $$\left[\hat{X}^2,\hat{P}_x^2\right]=\hat{X}\left[\hat{X},\hat{P}_x^2\right]+\left[\hat{X},\hat{P}_x^2\right]\hat{X}\Rightarrow\hat{X}2i\hbar\hat{P}_x+2i\hbar\hat{P}_x\hat{X}=2i\hbar\left(\hat{X}\hat{P}_x+\hat{P}_x\hat{X}\right)$$

Example: If $\hat{A}=a\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$ $\quad \hat{B}=b\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$

(a) Find the value of $[\hat{A},\hat{B}]$

(b) Write down eigen vector of $\hat{B}$ in the basis of eigen vector of A.

Solution: (a) $[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}=a\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}b\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}-b\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}a\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$

$=ab\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}-ba\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix}$ $[\hat{A},\hat{B}]$ so A and B commute.

(b) Eigen vector of A is $|a_1\rangle=\begin{pmatrix}1\\ 0\end{pmatrix}$ eigen value $\lambda_1=a$

$|a_2\rangle=\begin{pmatrix}0\\ 1\end{pmatrix}$ eigen value $\lambda_2=a$

Eigen vector of B is $|b_1\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}$ eigen value $\lambda_1=b$

$|b_2\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}$ eigen value $\lambda_{2\partial}=-b$

$$|b_1\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 0\end{pmatrix}+\frac{1}{\sqrt{2}}\begin{pmatrix}0\\ 1\end{pmatrix}=\frac{1}{\sqrt{2}}|a_1\rangle+\frac{1}{\sqrt{2}}|a_2\rangle$$

$$|b_2\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 0\end{pmatrix}-\frac{1}{\sqrt{2}}\begin{pmatrix}0\\ 1\end{pmatrix}\qquad |b_2\rangle=\frac{1}{\sqrt{2}}|a_1\rangle-\frac{1}{\sqrt{2}}|a_2\rangle$$

Example: For the symmetric potential i.e. $V(-x)=V(x)$, prove that parity operator $\hat{\pi}$ commute with Hamiltonian $\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)$.

Solution: $\left[\hat{H},\hat{\pi}\right]\psi(x)=\hat{H}\hat{\pi}\psi(x)-\hat{\pi}\hat{H}\psi(x)=\hat{H}\psi(-x)-\pi\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)\right)$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial(x)^2}+V(x)\psi(-x)-\pi\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)\right)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial(x)^2}+V(x)\psi(-x)-\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial(-x)^2}+V(-x)\psi(-x)\right)$$

Hence $V(-x)=V(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial x^2}+V(x)\psi(-x)\right)-\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial x^2}+V(x)\psi(-x)\right)=0$

$\left[\hat{H},\hat{\pi}\right]\psi(x)=0\Rightarrow\left[\hat{H},\hat{\pi}\right]=0$

$\hat{L}_z=\hat{X}\hat{P}_y-\hat{Y}\hat{P}_x$, find the value of $\left[\hat{X},\hat{L}_z\right]$ and $\left[\hat{P}_y,\hat{L}_z\right]$.

$$\left[\hat{X},\hat{L}_z\right]=\left[\hat{X},\hat{X}\hat{P}_y-\hat{Y}\hat{P}_x\right]=\left[\hat{X},\hat{X}\right]\hat{P}_y+\hat{X}\left[\hat{X},\hat{P}_y\right]-\left[\hat{X},\hat{Y}\right]\hat{P}_x-\hat{Y}\left[\hat{X},\hat{P}_x\right]$$

$$=0+0-0-i\hbar\hat{Y}=-i\hbar\hat{Y}$$

$$\left[\hat{P}_y,\hat{L}_z\right]=\left[\hat{P}_y,\hat{X}\hat{P}_y\right]-\left[\hat{P}_y,\hat{Y}\hat{P}_x\right]=0-(-i\hbar)\hat{P}_x=+i\hbar\hat{P}_x$$

Example: Given the usual canonical commutation relations, the commutator $[A,B]$ of $A=i\left(xp_y+yp_x\right)$ and $B=\left(yp_z+zp_y\right)$. Find the value of $[A,B]$.

Solution: $[A,B]=\left[\left(ixp_y+iyp_x\right),\left(yp_z+zp_y\right)\right]$

$$[A,B]=i\left[xp_y,yp_z\right]+i\left[yp_x,yp_z\right]+i\left[xp_y,zp_y\right]+i\left[yp_x,zp_y\right]$$

$$[A,B]=i\left[xp_y,yp_z\right]+0+0+i\left[yp_x,zp_y\right]=i\left[xp_y,yp_z\right]+i\left[yp_x,zp_y\right]$$

$$[A,B]=ix\left[p_y,yp_z\right]+i\left[x,yp_z\right]p_y+iy\left[p_x,zp_y\right]+i\left[y,zp_y\right]p_x$$

$$[A,B]=ix\left[p_y,yp_z\right]+0+0+i\left[y,zp_y\right]p_x=ix\left[p_y,yp_z\right]+i\left[y,zp_y\right]p_x$$

$$[A,B]=ix\times(-i\hbar)p_z+izi\hbar\times p_x$$

$$[A,B]=\hbar\left(xp_z-p_xz\right)$$

Example: Let x and p denote, respectively, the coordinate and momentum operators satisfying the canonical commutation relation $[x,p]=i$ in natural units $(\hbar=1)$. Then the commutator find commutator $[x,\ p\sin p]$ is

Solution: $\because [x,p]=i$

$$[x,\ p\sin p]=[x,p]\sin p+p[x,\sin p]=i\sin p+p\left[x,p-\frac{p^3}{\lfloor 3}....\right]$$

$$=i\sin p+p\left[[x,p]-\left[x,\frac{p^3}{\lfloor 3}\right]....\right]=i\sin p+p\left[i-\frac{3ip^2}{\lfloor 3}......\right]$$

$$\Rightarrow[x,p\sin p]\ =i\sin p+p\left[i-\frac{3ip^2}{\lfloor 3}......\right]=i\sin p+p\left[i+\frac{ip^2}{\lfloor 2}......\right]=i(\sin p+p\cos p)$$