College of Science
Department of Physics
Fourth Class
Lecture 7

Quantum Mechanics

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Lecture 7: Hermitian operator

Preparation

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3.7 Hermitian operator

The operators of interest in Q.M. fall into a special class of operators called Hermitian.

An operator $\hat{A}$ is said to be Hermitian if its expectation value in any normalized state Ψ is real

$$\bar{a} = \frac{\int \Psi^* \hat{A}\, \Psi dv}{\int \Psi^* \Psi dv}$$

i.e. $\boxed{\int_{-\infty}^{\infty} \Psi_1^* \hat{A} \Psi_2 d\vartheta = \int \Psi_2 \hat{A}^*\ \Psi_1^* d\vartheta}$

or $\boxed{\int_{-\infty}^{\infty} \Psi_1^* \hat{A} \Psi_2 d\vartheta = \int \hat{A}^* \Psi_1^* \Psi_2\ d\vartheta}$

where Ψ_1 and Ψ_2 are normalized eigen functions.

Also, an operator $\hat{A}$ is said to be Hermitian if it is equal to its adjoint $\hat{A}^\dagger$ or $(\hat{A} = \hat{A}^\dagger)$ or

$$\langle \Psi | \hat{A} | \emptyset \rangle = \langle \emptyset | \hat{A} | \Psi \rangle^*$$

Note: $\langle \boldsymbol{\Psi} |$ ***bra vector*** $\quad | \emptyset \rangle$ ***ket vector***

$\langle \boldsymbol{\Psi} | \boldsymbol{\Phi} \rangle$ ***Inner product***

Hilbert spaces: هو فضاء يحقق شروط الضرب الداخلي اوجده العالم ديراك لتفسير الظواهر الكمية .

$\langle \Psi | \emptyset \rangle \neq 0\ (normalization)$ $\langle \Psi | \emptyset \rangle = 0\ (orthogonal)$

3.8 Properties of Hermitian operators

<u>i- Every eigen value of a Hermitian operator is real.</u>

<u>Proof</u>

Let Ψ be an eigen function of Hermitian operator $\hat{A}$ belonging to the eigen value λ . According to condition of Hermitian operator

$$\int_{-\infty}^{\infty} \Psi^* \hat{A} \Phi dx = \int \hat{A}^* \Psi^* \Phi\ dx$$

Putting ($\Phi = \Psi$) in the above relation, we get

$$\int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi dx = \int \hat{A}^* \Psi^* \Psi \, dx$$

$\hat{A}\Psi = \lambda\Psi$, λ = eigen value of operator $\hat{A}$ and Ψ eigen function

Hence

$$\int_{-\infty}^{\infty} \Psi^* \lambda \Psi dx = \int \lambda^* \Psi^* \Psi \, dx$$

$\therefore \lambda$ is a number, therefore

$$\lambda \int_{-\infty}^{\infty} \Psi^* \Psi dx = \lambda^* \int \Psi^* \Psi \, dx$$

And hence $\boxed{\lambda = \lambda^*}$

This is only possible if λ is real number. this proves that every Hermitian operator gives real eigen values.

ii- If two eigen functions (Ψ_1 &Ψ_2) operated by the same Hermitian operator give two eigen values, they will be orthogonal functions.

Proof:

Let $\hat{A}$ be any Hermitian operator, (Ψ_1&Ψ_2) be two eigen functions of operator $\hat{A}$.

If λ_1 & λ_2 are eigen values corresponding to Ψ_1&Ψ_2 of operator $\hat{A}$,then

$\hat{A}\Psi_1 = \lambda_1\Psi_1$, $\hat{A}\Psi_2 = \lambda_2\Psi_2$

$\int_{-\infty}^{\infty} \Psi_1^* \hat{A} \Psi_2 d\vartheta = \int \hat{A}^* \Psi_1^* \Psi_2 \, d\vartheta$ condition of Hermitian

$\int_{-\infty}^{\infty} \Psi_1^* \hat{A} \Psi_2 dx = \int \lambda_1^* \Psi_1^* \Psi_2 \, dx = \lambda_1^* \int \Psi_1^* \Psi_2 \, dx = \lambda_1 \int \Psi_1^* \Psi_2 \, dx$

$\therefore \lambda_1$ is real -------------(1)

Similarly

$$\int_{-\infty}^{\infty} \Psi_1^* \hat{A} \Psi_2 dx = \int \Psi_1^* \lambda_2 \Psi_2 \, dx = \lambda_2 \int \Psi_1^* \Psi_2 \, dx ----(2)$$

Now from eq1 & eq2

$$\int_{-\infty}^{\infty} \Psi_1^* \hat{A} \Psi_2 dx = \lambda_1 \int \Psi_1^* \Psi_2 \, dx = \lambda_2 \int \Psi_1^* \Psi_2 \, dx$$

Subtracting eq2 from eq1

$$\lambda_1 \int \Psi_1^* \Psi_2 \, dx - \lambda_2 \int \Psi_1^* \Psi_2 \, dx = \int \Psi_1^* \hat{A} \Psi_2 dx - \int \Psi_1^* \hat{A} \Psi_2 dx = 0$$

$(\lambda 1 - \lambda 2)(\int \Psi_1^* \Psi_2 \, dx) = 0$

$\lambda_1 - \lambda_2 \neq 0$ because λ_1 & λ_2 are different eigen values i.e. $\lambda_1 \neq \lambda_2$

$\therefore \int \Psi_1^* \Psi_2 dx = 0$

i.e. Ψ_1 and Ψ_2 are orthogonal functions mutually.

iii- If $\hat{A}$ *and* $\hat{B}$ are commuting Hermitian operators, then the operator $\widehat{AB}$ is also Hermitian.

Proof:

To prove this, we write

$$\int \Psi^* \widehat{AB} \Phi dx = \int \Psi^* \hat{A} \big(\hat{B} \Phi \big) dx$$

$\hat{A}$ is Hermitian, then

$$\int \Psi^* \hat{A} (\hat{B} \Phi) dx = \int \hat{A}^* \Psi^* \big(\hat{B} \Phi \big) dx$$

$\hat{B}$ is also Hermitian, then

$\int \hat{A}^* \Psi^* \hat{B} \Phi$ dx= $\int \hat{B}^* \hat{A}^* \Psi^* \Phi$ dx

$\hat{A}$ *and* $\hat{B}$ are both Hermitian, then

$\int \Psi^* \widehat{AB} \Phi dx = \int \hat{B}^* A^* \Psi^* \Phi$ dx

$= \int (BA)^* \Psi^* \Phi dx ----(3)$

$\hat{A} \& \hat{B}$ *commute*

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

Substitute this into eq.3, then

$$\int \Psi^* \widehat{AB} \Phi dx = \int (AB)^* \Psi^* \Phi dx$$

According to definition of Hermitian operator

$$\int_{-\infty}^{\infty} \Psi^* \hat{A} \Phi dx = \int \hat{A}^* \Psi^* \Phi \, dx$$

Then AB is Hermitian operator

3.9 Linear operator in quantum mechanics

In Q.M. we are concerned almost exclusively with linear operator.

An operator $\hat{T}$ is said to be linear

1- If it commutes with constants, i.e.
$\hat{T}C = C\hat{T}$, C is constant
2- Obeys the distributive law $\hat{T}(\Psi + \Phi) = \hat{T}\Psi + \hat{T}\Phi$

3.10 Problems

Problem 1

In its lowest energy state, the eigen function of a S.H.O. satisfies

$$\Psi \propto \exp\left(\frac{-kx^2}{2}\right)$$

What is the correctly normalized eigen function?

Solution:

let the normalizing constant, N

$$\therefore \Psi = N exp\left(\frac{-kx^2}{2}\right)$$

Ψ is real

Ψ*Ψ= $N^2 exp\left(\frac{-kx^2}{2}\right) exp\left(\frac{-kx^2}{2}\right)$

=$N^2 exp\left(-kx^2\right)$

$$\int_{-\infty}^{\infty} \Psi^* \Psi dx = N^2 \int_{-\infty}^{\infty} \exp(-kx^2) \, dx$$

Let $y^2 = kx^2$ so $y = \sqrt{k}x$ than change the variable to $y = \sqrt{k}x$

$$\therefore dy = \sqrt{k} dx$$

$\int_{-\infty}^{\infty} \Psi^* \Psi dx = \frac{N^2}{\sqrt{k}} \int_{-\infty}^{\infty} \exp(-y^2) \, dy$

This integration can be found in tables of integrals. It would be always given, and its value is $\sqrt{\pi}$

$$\int_{-\infty}^{\infty} \Psi^* \Psi dx = \frac{N^2}{\sqrt{k}} \sqrt{\pi}$$

For normalized eigen function $\int_{-\infty}^{\infty} \Psi^* \Psi dx = 1$

$\therefore \frac{N^2}{\sqrt{k}} \sqrt{\pi} = 1$ so $N^2 = \sqrt{\frac{k}{\pi}}$ $\rightarrow N = (\frac{k}{\pi})^{\frac{1}{4}}$

Therefore, normalized eigen function, is

$$\Psi = (\frac{k}{\pi})^{\frac{1}{4}} exp(\frac{-kx^2}{2})$$

Problem 2

Calculate the expectation value of (P_x) for a particle associated with the wave function

$$\Psi = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) , \quad \frac{-a}{2} < x < \frac{a}{2}$$

Solution:

$P_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$

For normalized w.f.

$$\langle \hat{A} \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A}\, \Psi dx$$

$$\langle P_x \rangle = \int_{\frac{-a}{2}}^{\frac{a}{2}} \sqrt{\frac{2}{a}} \sin(\frac{2\pi x}{a}) \left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right) \sqrt{\frac{2}{a}}\, sin\left(\frac{2\pi x}{a}\right) dx$$

$$\langle P_x \rangle = \frac{2}{a} \frac{\hbar}{i} \int_{\frac{-a}{2}}^{\frac{a}{2}} \sin(\frac{2\pi x}{a}) \frac{\partial}{\partial x}\, sin\left(\frac{2\pi x}{a}\right) dx$$

$$\langle P_x \rangle = \frac{2}{a} \frac{\hbar}{i} \int_{\frac{-a}{2}}^{\frac{a}{2}} \sin(\frac{2\pi x}{a}) \cos\left(\frac{2\pi x}{a}\right). \frac{2\pi}{a}\, dx$$

Let $u = \frac{2\pi x}{a}$ $\rightarrow$ $du = \frac{2\pi}{a} dx$

Where $u = \frac{2\pi x}{a}$ $\quad where \quad x = \frac{a}{2}$

$\therefore u = \frac{2\pi}{a} \frac{a}{2} = \pi \ \rightarrow u = \pi$

And where $x = -\frac{a}{2}$

$\therefore u = \frac{2\pi}{a} \frac{-a}{2} \ \rightarrow u = -\pi$

$$\langle P_x \rangle = \frac{2}{a}\frac{\hbar}{i}\int_{-\pi}^{\pi} \sin u \ \cos u \ du \ = \frac{2}{a}\frac{\hbar}{i} 2\int_{0}^{\pi} \sin u \ \cos u \ du$$

$$= \frac{4}{a}\frac{\hbar}{i}\frac{sin^2 u}{2}\Big|_0^{\pi} = \frac{4}{a}\frac{\hbar}{i}(zero) = 0$$

Problem 3

$$\Psi(x,t) = Ae^{-\lambda|x|}e^{i\omega t}$$

Let A a normalization const

$$\Psi(x,t) = Ae^{-\lambda|x|}e^{i\omega t}$$

$$\int \Psi^* \Psi \, dx = \int |\Psi(x,t)|^2 \, dx = 1$$

$$\int |\Psi(x,t)|^2 \, dx = \int A\, e^{-\lambda|x|}e^{-i\omega t} \, Ae^{-\lambda|x|}e^{i\omega t} dx$$

$$= A^2 \int_{-\infty}^{\infty} e^{-2\lambda|x|} dx = 1$$

$$1 = 2A^2 \int_0^{\infty} e^{-2\lambda|x|} dx$$

$$1 = 2A^2 \frac{e^{-2\lambda x}}{-2\lambda}\Big|_0^{\infty} = \frac{2A^2}{-2\lambda}\left[e^{-2\lambda x}\right]_0^{\infty}$$

$1 = \frac{-A^2}{\lambda}(0-1) = \frac{A^2}{\lambda}$

$$\therefore A^2 = \lambda \ \rightarrow A = \sqrt{\lambda}$$

$$\Psi(x,t) = \sqrt{\lambda} e^{-\lambda|x|}e^{i\omega t}$$

Problem 4:

$$\psi(x) = A\left(ax - x^2\right) \text{ for } 0 \leq x \leq a$$

(a) Normalize the wavefunction

(b) Find $\langle x \rangle$, $\langle x^2 \rangle$

SOLUTION

(a) The wavefunction is real. So $\psi^*\psi = \psi^2$ and we have:

$$\int \psi^2 dx = \int_0^a A^2(ax - x^2)^2 dx = A^2 \int_0^a a^2x^2 - 2ax^3 + x$$

$$= A^2\left[a^2(x^3/3) - ax^4/2 + x^5/5\right]\Big|_0^a$$

$$= A^2\left[a^5/3 - a^5/2 + a^5/5\right]$$

$$= A^2\left[10a^5/30 - 15a^5/30 + 6a^5/30\right]$$

$$= A^2a^5/30, \Rightarrow A = \sqrt{30/a^5}$$

(b)

$$\langle x \rangle = \int x^2\psi^2 dx = (30/a^5)\int_0^a x(ax - x^2)^2 dx$$

$$= (30/a^5)\int_0^a a^2x^3 - 2ax^4 + x^5 dx$$

$$= (30/a^5)\left[a^2\left(x^4/4\right) - 2a\left(x^5/5\right) + x^6/6\right]\Big|_0^a$$

$$= (30/a^5)\left[a^6/4 - 2a^6/5 + a^6/6\right]$$

$$= (30/a^5)(a^2/60) = \frac{a}{2}$$

$$\langle x^2 \rangle = \int x^2\psi^2 dx = (30/a^5)\int_0^a x^2\left(ax - x^2\right)^2 dx$$

$$= (30/a^5)\int_0^a a^2x^4 - 2ax^5 + x^6 dx$$

$$= (30/a^5)\left[a^2\left(x^5/5\right) - 2a\left(x^6 + x^7/7\right)\right]\Big|_0^a$$

$$= (30/a^5)\left[a^2\left(x^5/5\right) - 2a\left(x^6 + x^7/7\right)\right]\Big|_0^a$$

$$= (30/a^5)\left[a^7/5 - 2a^7/6 + a^7/7\right]$$

$$= \frac{2a^2}{7}$$