

## **PH107 D1T5: Tutorial 5**

*12-01-2022*

# OPERATORS AND WAVE FUNCTION

## Question 1

Which of the operators  $A_i$  defined in the following are linear operators? Which of these are hermitian? All the functions  $\psi(x)$  are well behaved functions vanishing at  $\pm\infty$ .

(a)  $\hat{A}_1\psi(x) = \psi(x)^2$

$$\begin{aligned}\hat{A}_1 c\psi(x) &= (c\psi(x))^2 \\ &= c^2\psi(x)^2 \\ &= c^2\hat{A}_1\psi(x)\end{aligned}\tag{1}$$

Not a linear Operator

The operator  $\hat{A}_1$  is called hermitian if  $\int (\hat{A}_1\psi)^*\psi dx = \int \psi^*\hat{A}_1\psi dx$

$$\begin{aligned}\implies LHS &= \int (\psi^2)^*\psi dx \\ &\implies \neq RHS\end{aligned}\tag{2}$$

Not a Hermitian

(b)  $\hat{A}_2\psi(x) = \frac{\partial\psi(x)}{\partial x}$

$$\begin{aligned}\hat{A}_2 c\psi(x) &= \frac{\partial c\psi(x)}{\partial x} \\ &= c \frac{\partial\psi(x)}{\partial x} \\ &= c\hat{A}_2\psi(x) \\ \hat{A}_2(\psi(x) + \phi(x)) &= \frac{\partial(\psi(x) + \phi(x))}{\partial x} \\ &= \frac{\partial\psi(x)}{\partial x} + \frac{\partial\phi(x)}{\partial x} \\ &= \hat{A}_2\psi(x) + \hat{A}_2\phi(x)\end{aligned}\tag{3}$$

Linear Operator

The operator  $\hat{A}_2$  is called hermitian if  $\int (\hat{A}_2\psi)^*\psi dx = \int \psi^*\hat{A}_2\psi dx$

$$\implies LHS = \int \left(\frac{\partial\psi(x)}{\partial x}\right)^* \psi(x) dx\tag{4}$$

Using Integration by parts and  $\psi$  tends to zero as  $x \rightarrow \infty$

$$\begin{aligned} &= - \int \left( \frac{\partial \psi(x)}{\partial x} \right) \psi(x)^* dx \\ &= -RHS \end{aligned} \quad (5)$$

Not a Hermitian

(c)  $\hat{A}_3 \psi(x) = \int_a^x \psi(x') dx'$

$$\begin{aligned} \hat{A}_3 c\psi(x) &= \int_a^x c\psi(x') dx' \\ &= c \int_a^x \psi(x') dx' \\ &= c \hat{A}_3 \psi(x) \\ \hat{A}_3(\psi(x) + \phi(x)) &= \int_a^x (\psi(x') + \phi(x')) dx' \\ &= \int_a^x \psi(x') dx' + \int_a^x \phi(x') dx' \\ &= \hat{A}_3 \psi(x) + \hat{A}_3 \phi(x) \end{aligned} \quad (6)$$

Linear Operator

The operator  $\hat{A}_3$  is called hermitian if  $\int (\hat{A}_3 \psi)^* \psi dx = \int \psi^* \hat{A}_3 \psi dx$

$$\begin{aligned} LHS &= \int \left( \int_a^x \psi \right)^* \psi dx \\ &= \int \left( \int_a^x \psi^* \right) \psi dx \\ &\neq \int \psi^* \left( \int_a^x \psi \right) dx \end{aligned} \quad (7)$$

Not Hermitian

(d)  $\hat{A}_4 \psi(x) = 1/\psi(x)$

$$\begin{aligned} \hat{A}_4 c\psi(x) &= \frac{1}{c\psi(x)} \\ &= \frac{1}{c} \hat{A}_4 \psi(x) \end{aligned} \quad (8)$$

Not a linear Operator

The operator  $\hat{A}_4$  is called hermitian if  $\int (\hat{A}_4\psi)^*\psi dx = \int \psi^* \hat{A}_4\psi dx$

$$\int \frac{1}{\psi^*} \psi dx \neq \int \psi^* \frac{1}{\psi} dx \quad (9)$$

Not Hermitian

(e)  $\hat{A}_5\psi(x) = -\psi(x+a)$

$$\begin{aligned} \hat{A}_5 c\psi(x) &= -c\psi(x+a) \\ &= c\hat{A}_5\psi(x) \\ \hat{A}_5(\psi(x) + \phi(x)) &= -(\psi(x+a) + \phi(x+a)) \\ &= \hat{A}_5\psi(x) + \hat{A}_5\phi(x) \end{aligned} \quad (10)$$

Linear Operator

The operator  $\hat{A}_5$  is called hermitian if  $\int (\hat{A}_5\psi)^*\psi dx = \int \psi^* \hat{A}_5\psi dx$

$$\int -\psi(x+a)^*\psi dx \neq \int \psi^* -\psi(x+a) dx \quad (11)$$

Not Hermitian

(f)  $\hat{A}_6\psi(x) = \sin(\psi(x))$

$$\begin{aligned} \hat{A}_6 c\psi(x) &= \sin(c\psi(x)) \\ &\neq c\hat{A}_6\psi(x) \end{aligned} \quad (12)$$

Not Linear Operator

The operator  $\hat{A}_6$  is called hermitian if  $\int (\hat{A}_6\psi)^*\psi dx = \int \psi^* \hat{A}_6\psi dx$

$$\int \sin(\psi(x))\psi dx \neq \int \psi^* \sin(\psi(x)) dx \quad (13)$$

Not Hermitian

(g)  $\hat{A}_7\psi(x) = \frac{\partial^2 \psi(x)}{\partial x^2}$

$$\begin{aligned}
\hat{A}_7 c\psi(x) &= \frac{\partial^2 c\psi(x)}{\partial x^2} \\
&= c \frac{\partial^2 \psi(x)}{\partial x^2} \\
&= c \hat{A}_7 \psi(x) \\
\hat{A}_7(\psi(x) + \phi(x)) &= \frac{\partial^2(\psi(x) + \phi(x))}{\partial x^2} \\
&= \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{\partial^2 \phi(x)}{\partial x^2} \\
&= \hat{A}_7 \psi(x) + \hat{A}_7 \phi(x)
\end{aligned} \tag{14}$$

Linear Operator

The operator  $\hat{A}_7$  is called hermitian if  $\int (\hat{A}_7 \psi)^* \psi dx = \int \psi^* \hat{A}_7 \psi dx$

$$\begin{aligned}
LHS &= \int \left( \frac{\partial^2 \psi(x)}{\partial x^2} \right)^* \psi(x) dx \\
&= - \int \left( \frac{\partial \psi(x)}{\partial x} \right)^* \left( \frac{\partial \psi(x)}{\partial x} \right) dx \\
&= \int \psi(x)^* \left( \frac{\partial^2 \psi(x)}{\partial x^2} \right) dx \\
&= RHS
\end{aligned} \tag{15}$$

Hermitian

## Question 2

(a) If  $\hat{A}$  and  $\hat{B}$  are Hermitian and  $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = i\hat{C}$ , prove that  $\hat{C}$  is Hermitian

$$\begin{aligned}
\hat{A}\hat{B} - \hat{B}\hat{A} &= i\hat{C} \\
\Rightarrow (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger &= -i\hat{C}^\dagger \\
\Rightarrow (\hat{A}\hat{B})^\dagger - (\hat{B}\hat{A})^\dagger &= -i\hat{C}^\dagger \\
\Rightarrow \hat{B}^\dagger \hat{A}^\dagger - \hat{A}^\dagger \hat{B}^\dagger &= -i\hat{C}^\dagger \\
\hat{B}\hat{A} - \hat{A}\hat{B} &= -i\hat{C}^\dagger \\
-i\hat{C} &= -i\hat{C}^\dagger \\
\hat{C} &= \hat{C}^\dagger
\end{aligned} \tag{16}$$

(b) An operator is said to be anti-Hermitian if  $\hat{O}^\dagger = -\hat{O}$ . Prove that  $[\hat{A}, \hat{B}]$  is antiHermitian.

$$\begin{aligned}
 [\hat{A}, \hat{B}]^\dagger &= (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger \\
 &= (\hat{A}\hat{B})^\dagger - (\hat{B}\hat{A})^\dagger \\
 &= \hat{B}^\dagger \hat{A}^\dagger - \hat{A}^\dagger \hat{B}^\dagger \\
 &= \hat{B}\hat{A} - \hat{A}\hat{B} \\
 &= -[\hat{A}, \hat{B}]
 \end{aligned} \tag{17}$$

### Question 3

Prove that if  $\hat{K}$  is a Hermitian operator,  $\exp(i\hat{K})$  is an unitary operator, and if  $\hat{U}$  is an Unitary operator, then there is an operator  $K$  such that  $\hat{U} = \exp(i\hat{K})$  and this  $\hat{K}$  is Hermitian.

Given,  $\hat{K}$  is Hermitian. Let,  $\hat{U} = \exp(i\hat{K})$

$$\begin{aligned}
 \hat{U} \cdot \hat{U}^\dagger &= \exp(i\hat{K}) \exp(-i\hat{K}^\dagger) \\
 &= \exp(i(\hat{K} - \hat{K}^\dagger)) \\
 &= 1
 \end{aligned} \tag{18}$$

Given,  $\hat{U}$  is unitary. Then, by the Spectral Theorem for unitary matrices, there is another **unitary matrix**  $B$  such that  $U = B\Lambda B^{-1}$ , and  $\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$ . As all  $|\lambda_k| = 1$ , we write them as  $\lambda_k = e^{i\theta_k}$  where  $\theta_k$  are real numbers. Then set

$$A = B \text{diag}(\theta_1, \theta_2, \dots, \theta_n) B^{-1} = B\Lambda_1 B^{-1}$$

Then  $A$  is Hermitian:

$$A^\dagger = (B^{-1})^\dagger \Lambda_1 B^\dagger = B\Lambda_1 B^{-1} = A,$$

and evidently  $\exp(iA) = U$

### Question 4

If  $\hat{A}$  and  $\hat{B}$  are operators, prove

(a) that  $(\hat{A}^\dagger)^\dagger = \hat{A}$

$A^\dagger$  is transpose conjugate of  $A$ . So, taking transpose-conjugate twice will not change matrix.

$$(\hat{A}^\dagger)^\dagger = \hat{A}$$

(b) that  $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$

$$\begin{aligned}\int \phi^* \hat{A}\hat{B}\psi &= \int (\hat{A}^\dagger\phi)^* \hat{B}\psi = \int (\hat{B}^\dagger\hat{A}^\dagger\phi)^* \psi \\ (\hat{A}\hat{B})^\dagger &= \hat{B}^\dagger\hat{A}^\dagger\end{aligned}\quad (19)$$

(c) that  $\hat{A} + \hat{A}^\dagger$ ,  $i(\hat{A} - \hat{A}^\dagger)$ , and that  $\hat{A}\hat{A}^\dagger$  are Hermitian operators.

An operator  $\hat{A}$  is Hermitian if  $\hat{A} = \hat{A}^\dagger$

$$\begin{aligned}(\hat{A} + \hat{A}^\dagger)^\dagger &= (\hat{A}^\dagger + \hat{A}) \\ i(\hat{A} - \hat{A}^\dagger)^\dagger &= -i(\hat{A}^\dagger - \hat{A}) \\ &= i(\hat{A} - \hat{A}^\dagger)^\dagger \\ (\hat{A}\hat{A}^\dagger)^\dagger &= (\hat{A}^\dagger)^\dagger \hat{A}^\dagger \\ &= \hat{A}\hat{A}^\dagger\end{aligned}\quad (20)$$

## Question 5

An operator is given by

$$\hat{G} = i\hbar \frac{\partial}{\partial x} + Bx$$

where  $B$  is a constant. Find the eigen function  $\phi(x)$ . If this eigen function is subjected to a boundary condition  $\phi(a) = \phi(-a)$  find out the eigen values.

We need to solve the differential equation

$$\begin{aligned}\hat{G}\phi(x) &= \lambda\phi(x) \\ \implies i\hbar \frac{d\phi(x)}{dx} + Bx\phi(x) &= \lambda\phi(x) \\ \implies \frac{d\phi(x)}{dx} &= \frac{i}{\hbar}(Bx - \lambda)\phi(x) \\ \implies \int \frac{1}{\phi(x)} d\phi(x) &= \frac{i}{\hbar} \int (Bx - \lambda) dx \\ \implies \ln \phi(x) &= \frac{i}{\hbar} \left( \frac{B}{2}x^2 - \lambda x \right) + \ln(C) \\ \implies \phi(x) &= Ce^{-i\frac{\lambda}{\hbar}x} e^{i\frac{B}{2\hbar}x^2}\end{aligned}\quad (21)$$

Applying the boundary condition  $\phi(a) = \phi(-a)$

$$\begin{aligned}\implies e^{i\frac{2a\lambda}{\hbar}} &= 1 \\ \implies \frac{2a\lambda}{\hbar} &= 2n\pi, n \in \mathcal{N} \\ \implies \lambda_n &= \frac{n\pi\hbar}{a}\end{aligned}\quad (22)$$

## Question 6

$\psi_1(x)$  and  $\psi_2(x)$  are the normalized eigen functions of an operator  $\hat{P}$ , with eigen values  $P_1$  and  $P_2$  respectively. If the wave function of a particle is  $0.25\psi_1(x) + 0.75\psi_2(x)$  at  $t = 0$ , find the probability of observing  $P_1$

Since  $\hat{P}$  corresponds to an observable, therefore it is a Hermitian Operator. Thus it's eigen-functions with distinct eigenvalues must be orthogonal

$$\langle \psi_1 | \psi_2 \rangle = \langle \psi_2 | \psi_1 \rangle = 0$$

$$\langle \psi_1 | \psi_1 \rangle = \langle \psi_2 | \psi_2 \rangle = 1$$

According to the postulates of QM, the probability of observing  $P_1$  is  $\frac{|\langle \psi_1 | \psi \rangle|^2}{\langle \psi | \psi \rangle}$  where  $\psi(x) = 0.25\psi_1(x) + 0.75\psi_2(x)$

$$\langle \psi_1 | \psi \rangle = 0.25 \langle \psi_1 | \psi_1 \rangle + 0.75 \langle \psi_1 | \psi_2 \rangle = 0.25$$

$$\begin{aligned} \langle \psi | \psi \rangle &= 0.25^2 \langle \psi_1 | \psi_1 \rangle + 0.75^2 \langle \psi_2 | \psi_2 \rangle + 0.25 * 0.75 \langle \psi_1 | \psi_2 \rangle + 0.25 * 0.75 \langle \psi_2 | \psi_1 \rangle \quad (23) \\ &= 0.25^2 + 0.75^2 \end{aligned}$$

$$\text{Probability of } P_1 = \frac{|\langle \psi_1 | \psi \rangle|^2}{\langle \psi | \psi \rangle} = \frac{0.25^2}{0.25^2 + 0.75^2} = \frac{1}{10} = 0.1$$

## Question 7

Consider a large number ( $N$ ) of identical experimental set-ups. In each of these, a single particle is described by a wave function  $\Phi(x) = A \exp(-x^2/b^2)$  at  $t = 0$ , where  $A$  is the normalization constant and  $b$  is another constant with the dimension of length. If a measurement of the position of the particle is carried out at time  $t = 0$  in all these set-ups, it is found that in 100 of these, the particle is found within an infinitesimal interval of  $x = 2b$  to  $2b + dx$ . Find out, in how many of the measurements, the particle would have been found in the infinitesimal interval of  $x = b$  to  $b + dx$ .

$$\begin{aligned} \frac{N_{[2b, 2b+dx]}}{N_{[b, b+dx]}} &= \frac{P(2b < x < 2b + dx)}{P(b < x < b + dx)} \\ &= \frac{|\phi(2b)|^2 dx}{|\phi(b)|^2 dx} = e^{-\frac{4b^2 - b^2}{b^2}} = e^{-6} \quad (24) \\ \Rightarrow N_{[b, b+dx]} &\approx 100e^6 \approx 40343 \end{aligned}$$

## Question 8

An observable  $A$  is represented by the operator  $\hat{A}$ . Two of its normalized eigen functions are given as  $\Phi_1(x)$  and  $\Phi_2(x)$ , corresponding to distinct eigenvalues  $a_1$  and  $a_2$ , respectively. Another observable  $B$  is represented by an operator  $\hat{B}$ . Two normalized eigen functions of this operator are given as  $u_1(x)$  and  $u_2(x)$  with distinct eigenvalues  $b_1$  and  $b_2$ , respectively. The eigen functions



$\Phi_1(x)$  and  $\Phi_2(x)$  are related to  $u_1(x)$  and  $u_2(x)$  as,  $\Phi_1 = D(3u_1 + 4u_2)$ ;  $\Phi_2 = F(4u_1 - Pu_2)$  At time  $t = 0$ , a particle is in a state given by  $\frac{2}{3}\Phi_1 + \frac{1}{3}\Phi_2$ .

(a) Find the values of  $D$ ,  $F$  and  $P$

We know that  $\Phi_1, \Phi_2, u_1, u_2$  are normalized, and  $\Phi_1, \Phi_2$  are orthogonal and so are  $u_1, u_2$ .

$$\begin{aligned}
 \langle \Phi_1 | \Phi_1 \rangle &= 1 \\
 \Rightarrow 25|D|^2 &= 1 \\
 \Rightarrow D &= 0.2e^{i\theta} \\
 \langle \Phi_1 | \Phi_2 \rangle &= 0 \\
 \Rightarrow \bar{D}F(12\langle u_1 | u_1 \rangle - 4P\langle u_2 | u_2 \rangle - 3P\langle u_1 | u_2 \rangle + 16\langle u_2 | u_1 \rangle) &= 0 \\
 \Rightarrow P &= 3 \\
 \langle \Phi_2 | \Phi_2 \rangle &= 1 \\
 \Rightarrow |F|^2(16\langle u_1 | u_1 \rangle + 9\langle u_2 | u_2 \rangle - 12\langle u_2 | u_1 \rangle - 12\langle u_1 | u_2 \rangle) &= 1 \\
 \Rightarrow 25|F|^2 &= 1 \\
 \Rightarrow F &= 0.2e^{i\theta}
 \end{aligned} \tag{25}$$

(b) If a measurement of  $A$  is carried out at  $t = 0$ , what are the possible results and what are their probabilities ?

According to the postulates of QM, the possible results of an  $A$  measurement are the eigenvalues  $a_1$  and  $a_2$ , and the probability is  $\frac{|\langle \Phi | \psi \rangle|^2}{\langle \psi | \psi \rangle}$  where  $\Phi$  is the corresponding eigenfunction and  $\psi = \frac{2}{3}\Phi_1 + \frac{1}{3}\Phi_2$

$$\begin{aligned}
 \langle \Phi_1 | \psi \rangle &= \frac{2}{3} \\
 \langle \Phi_2 | \psi \rangle &= \frac{1}{3} \\
 \langle \psi | \psi \rangle &= \frac{4}{9} + \frac{1}{9} = \frac{5}{9}
 \end{aligned} \tag{26}$$

$$\Rightarrow \text{Probability}(a_1) = \frac{\frac{4}{9}}{\frac{5}{9}} = 0.8$$

$$\Rightarrow \text{Probability}(a_2) = \frac{\frac{1}{9}}{\frac{5}{9}} = 0.2$$

(c) Assume that the measurement of  $A$  mentioned above yielded a value  $a_1$ . If a measurement of  $B$  is carried out immediately after this, what would be the possible outcomes and what would be their probabilities ?

According to the postulates of QM, once  $a_1$  is measured, the wavefunction will collapse to  $\Phi_1$ . Thus the wavefunction at the moment after measurement is  $\Phi_1(x)$ . Again we repeat

the same exercise as above for  $u_1$  and  $u_2$ . The possible outcomes are of course  $b_1$  and  $b_2$ .

$$\begin{aligned}\langle u_1 | \Phi_1 \rangle &= 0.6e^{i\theta} \\ \langle u_2 | \Phi_1 \rangle &= 0.8e^{i\theta} \\ \langle \Phi_1 | \Phi_1 \rangle &= 1\end{aligned}\tag{27}$$

$$\Rightarrow \text{Probability}(b_1) = 0.36$$

$$\Rightarrow \text{Probability}(b_2) = 0.64$$

(d) If instead of following the above path, a measurement of  $B$  was carried out initially at  $t = 0$ , what would be the possible outcomes and what would be their probabilities?

Following same steps as above, the possible outcomes are same,  $b_1$  and  $b_2$

$$\begin{aligned}\psi &= \frac{2}{3}\Phi_1 + \frac{1}{3}\Phi_2 \\ &= \left(\frac{2}{5}e^{i\theta} + \frac{4}{15}e^{i\Phi}\right)u_1 + \left(\frac{8}{15}e^{i\theta} - \frac{1}{5}e^{i\Phi}\right)u_2 \\ \langle u_1 | \psi \rangle &= \frac{2}{5}e^{i\theta} + \frac{4}{15}e^{i\Phi} \\ \langle u_2 | \psi \rangle &= \frac{8}{15}e^{i\theta} - \frac{1}{5}e^{i\Phi} \\ \langle \psi | \psi \rangle &= \frac{5}{9}\end{aligned}\tag{28}$$

$$\text{Probability}(b_1) = \frac{9}{5} \left( \frac{4}{25} + \frac{16}{225} + 2\frac{8}{75} \cos(\theta - \Phi) \right)$$

$$\text{Probability}(b_2) = \frac{9}{5} \left( \frac{64}{225} + \frac{1}{25} - 2\frac{8}{75} \cos(\theta - \Phi) \right)$$

(e) Assume that after performing the measurements described in (c), the outcome was  $b_2$ . What would be the possible outcomes, if  $A$  were measured immediately after this and what would be the probabilities?

So immediately after measurement the wavefunction collapses to  $u_2$ . Now once again the possibilities are  $a_1$  and  $a_2$

$$\begin{aligned}\langle \Phi_1 | u_2 \rangle &= \langle u_2 | \Phi_1 \rangle^* = 0.8e^{-i\theta} \\ \langle \Phi_2 | u_2 \rangle &= \langle u_2 | \Phi_2 \rangle^* = -0.6e^{-i\Phi} \\ \langle u_2 | u_2 \rangle &= 1\end{aligned}\tag{29}$$

$$\text{Probability}(a_1) = 0.64$$

$$\text{Probability}(a_2) = 0.36$$