QM
Phys 651

Lecture # 6

1

Matrix representation of kets & bras

$$|\Psi\rangle = \sum_n a_n |\varphi_n\rangle \quad ; \quad a_n = \langle \varphi_n | \Psi\rangle$$

a_n ← complex number (projection of $|\Psi\rangle$ onto $|\varphi_n\rangle$).

⇓

So, within the basis $\{|\varphi_n\rangle\}$, the ket $|\Psi\rangle$ is <u>represented</u> by the set of its components $a_1, a_2, \ldots$ along $|\varphi_1\rangle, |\varphi_2\rangle, \ldots$, respectively.

⇓

$$|\Psi\rangle \doteq \begin{pmatrix} \langle \varphi_1|\Psi\rangle \\ \langle \varphi_2|\Psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

$\doteq$ ← "represented by" (in some texts "$\mapsto$" is used)

← generally, infinite number of components

$$\langle \Psi| \doteq \left(\langle \Psi|\varphi_1\rangle \; \langle \Psi|\varphi_2\rangle \ldots \right) =$$

$$= \left(\langle \varphi_1|\Psi\rangle^* \; \langle \varphi_2|\Psi\rangle^* \ldots \right) = \left(a_1^* \; a_2^* \ldots \right.$$

Then, a bra-ket $\langle\psi|\varphi\rangle \Rightarrow$

$$\langle\psi|\varphi\rangle \doteq \left(a_1^* \; a_2^* \; \ldots \; a_n^* \ldots\right)\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \\ \ldots \end{pmatrix} =$$

$$= \sum_n a_n^* b_n$$

Matrix representation of operators

$$A = I A I = \left(\sum_{n=1}^{\infty} |\varphi_n\rangle\langle\varphi_n|\right) A \left(\sum_{m=1}^{\infty} |\varphi_m\rangle\langle\varphi_m|\right) =$$

identity operator

$$= \sum_{n,m} A_{nm} |\varphi_n\rangle\langle\varphi_m| \, , \text{ where}$$

$$A_{nm} = \langle\varphi_n|A|\varphi_m\rangle$$

$$A \doteq \begin{pmatrix} A_{11} & A_{12} & A_{13} & \ldots \\ A_{21} & A_{22} & A_{23} & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots \end{pmatrix}$$

generally, an infinite number of columns and rows

$\Rightarrow$ operators are represented by square matrices

Note: if $|\varphi_n\rangle$ are eigenkets of $A \Rightarrow A_{nm} =$
$= \langle\varphi_n|\tilde{a}_m|\varphi_m\rangle = \tilde{a}_m \delta_{nm} \Rightarrow$ matrix is diagonal

- Hermitian adjoint operation in matrix representation

So, $(A)^{+} = A^{+}$ =>

$$A \doteq \begin{pmatrix} A_{11} & A_{12} & A_{13} & \dots \\ A_{21} & A_{22} & A_{23} & \dots \\ \dots & & & \end{pmatrix}, \quad A^{+} \doteq ?$$

$$A^{+} \doteq \begin{pmatrix} A_{11}^{*} & A_{21}^{*} & A_{31}^{*} & \dots \\ A_{12}^{*} & A_{22}^{*} & A_{32}^{*} & \dots \\ \vdots & \vdots & \vdots & \end{pmatrix}, \text{ i.e. } A_{nm}^{+} = A_{mn}^{*}$$

So, the matrix which represents the operator A^{+} is obtained by taking the complex conjugate of the matrix transpose of A.

If A is Hermitian => $A_{mn}^{*} = A_{nm}$

- Inverse matrix

$$A_{nm}^{-1} = \frac{\text{cofactor of } A_{mn}}{\det A}, \quad \text{cofactor of } A_{mn} = (-1)^{m+n} \cdot \det [\text{submatrix}]$$

submatrix obtained by removing m th row and n th column

- Matrix representation of $|\Psi\rangle\langle\Psi|$

$$|\Psi\rangle\langle\Psi| \doteq \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} \begin{pmatrix} a_1^* & a_2^* & a_3^* & \dots \end{pmatrix} =$$

$$= \begin{pmatrix} a_1 a_1^* & a_1 a_2^* & a_1 a_3^* & \dots \\ a_2 a_1^* & a_2 a_2^* & a_2 a_3^* & \dots \\ \dots & & & \end{pmatrix}$$

- Trace of an operator

$$Tr(A) = \sum_n \langle \varphi_n | A | \varphi_n \rangle = \sum_n A_{nn}$$

sometimes called $Sp(A)$

spur (german: trace)

$$Tr \begin{pmatrix} A_{11} & A_{12} & A_{13} & \dots \\ A_{21} & A_{22} & A_{23} & \dots \\ \dots & & & \end{pmatrix} = A_{11} + A_{22} + A_{33} + \dots$$

Properties of the trace

- Does not depend on the basis
- $Tr(A^+) = (Tr(A))^*$

- $\mathrm{Tr}(\alpha A + \beta B + \gamma C + \dots) =$
$= \alpha \,\mathrm{Tr}(A) + \beta\, \mathrm{Tr}(B) + \gamma\, \mathrm{Tr}(C) + \dots$

- $\mathrm{Tr}(ABCDE) = \mathrm{Tr}(EABCD) =$
$= \mathrm{Tr}(DEABC) = \dots$

invariant under the cyclic permutation

Summary of properties of a matrix A. The matrix A is:

- Real if $A = A^*$ or $A_{mn} = A^*_{mn}$
- Imaginary if $A = -A^*$ or $A_{mn} = -A^*_{mn}$
- Symmetric if $A = A^T$ or $A_{mn} = A_{nm}$
- Antisymmetric if $A = -A^T$ or $A_{mn} = -A_{nm}$, $A_{mm} = 0$
- Hermitian if $A = A^+$ or $A_{mn} = A^*_{nm}$
- Anti-Hermitian if $A = -A^+$ or $A_{mn} = -A^*_{nm}$
- Orthogonal if $A^T = A^{-1}$ or $(AA^T)_{mn} = \delta_{mn}$
- Unitary if $A^+ = A^{-1}$ or $(AA^+)_{mn} = \delta_{mn}$

Measurements. Eigenvalues and expectation values

Consider a system in a state $|\psi\rangle$. We would like to measure an observable A in this system. What would be our possible outcomes of the measurement? $\Rightarrow$

Present the state before the measurement, i.e. $|\psi\rangle$, in terms of eigenstates of an operator A corresponding to the observable we want to measure:
$$|\psi\rangle = \sum_n d_n |\varphi_n\rangle$$

The act of measurement (in general) changes the state of the system! - where to? $\Rightarrow$

one of the eigenstates $|\varphi_n\rangle$, and the result of the measurement is a_n.

If $|\psi\rangle$ is normalized, the probability to measure a_n and find the system in the state $|\varphi_n\rangle$ afterwards is $\underbrace{|\langle\varphi_n|\psi\rangle|^2}_{=|\alpha_n|^2}$ ⑦

If the system is initially in one of the eigenstates $|\varphi_k\rangle \Rightarrow$ the outcome will be a_k with probability 1.

Expectation value of A with respect to state $|\psi\rangle$ is $\bar{A} = \langle A \rangle = \langle A \rangle_\psi =$

normalised

different notations

$$= \langle \psi | A | \psi \rangle =$$

$$= \sum_{n,m} \langle \psi | \varphi_n \rangle \langle \varphi_n | \overbrace{A | \varphi_m \rangle}^{= a_m |\varphi_m\rangle} \langle \varphi_m | \psi \rangle =$$

$$= \sum_{n,m} a_m \langle \psi | \varphi_n \rangle \, \delta_{nm} \langle \varphi_m | \psi \rangle =$$

$$= \sum_n a_n \, |\langle \psi | \varphi_n \rangle|^2 = \sum_n a_n |\alpha_n|^2$$

measured value

probability of obtaining a_n

Mathematical analog of the "measurement" $\Rightarrow$ applying a projection operator $P_n|\Psi\rangle =$
$= |\varphi_n\rangle\langle\varphi_n|\Psi\rangle$

Analog of the expectation value $\Rightarrow$ weighted average

<u>Note</u>: • if $|\Psi\rangle$ is <u>not</u> normalized $\Rightarrow$

$$\langle A\rangle = \frac{\langle\Psi|A|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_n a_n \frac{|\langle\varphi_n|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle}$$

for a discrete spectrum of states

For a continuous spectra $\Rightarrow$

$$\langle A\rangle = \frac{\int a\,\mathcal{P}(a)\,da}{\int \underbrace{\mathcal{P}(a)}_{\text{probability density}}\,da}, \quad \mathcal{P}(a) = |\Psi(a)|^2$$

• The expectation value of an observable can be obtained physically as follows: prepare a large number of <u>identical</u> systems in the same state $|\Psi\rangle$ and measure the observable A in all these systems $\Rightarrow$ the results will be $a_1, a_2, \ldots$ with probabilities of occurrences $\mathcal{P}_1, \mathcal{P}_2 \ldots$ $\Rightarrow$ then $\langle A\rangle = \sum_n a_n \mathcal{P}_n$