Matrix Representation:

The ket $|\psi\rangle$ is represented by the set of numbers,

$$|\psi\rangle = a_n = \langle \phi_n|\psi\rangle$$

$$|\psi\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} \langle \phi_1|\psi\rangle \\ \langle \phi_2|\psi\rangle \\ \langle \phi_3|\psi\rangle \\ \vdots \end{pmatrix}$$

Let $\langle \chi|$ be an arbitrary bra

$$\langle \chi| = \langle \chi|\hat{I} = \sum_n \langle \chi|\phi_n\rangle\langle \phi_n|$$

$$= \sum_n \langle \phi_n|\chi\rangle^* \langle \phi_n|$$

$$= \sum_n b_n^* \langle \phi_n|$$

$$b_n = \langle \chi|\phi_n\rangle$$

or

$$\langle \chi| = \begin{pmatrix} b_1^* & b_2^* & b_3^* & \cdots \end{pmatrix} =$$

$$= \begin{pmatrix} \langle \phi_1|\chi\rangle & \langle \phi_2|\chi\rangle & \cdots \end{pmatrix}$$

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The scalar product is

$$\langle \chi|\psi\rangle = \langle \chi|\mathbb{1}|\psi\rangle$$

$$= \sum_n \langle \chi|\phi_n\rangle\langle \phi_n|\psi\rangle$$

$$= \sum_n b_n^* a_n$$

$\Rightarrow$

$$\langle \psi|\psi\rangle = \sum_n |a_n|^2 = 1 \geq 0$$

$\langle \psi|\psi\rangle$ is a number, $|\psi\rangle\langle\psi|$ is a matrix

$$|\psi\rangle\langle\psi| = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \begin{pmatrix} a_1^* & a_2^* & \cdots \end{pmatrix}$$

$$= \begin{pmatrix} a_1^* a_1 & a_1^* a_2 & \cdots \\ a_2^* a_1 & a_2^* a_2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

The matrix elements of an operator A are

$$A_{mn} = \langle \phi_m|A|\phi_n\rangle$$

where

$$A_{mn} = \langle \phi_m , A\phi_n \rangle = \int \phi_m^* \hat{A} \phi_n \, dx$$

The matrix elements can be arranged in a square matrix

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} \langle \phi_1, A\phi_1 \rangle & \langle \phi_1 , A\phi_2 \rangle & \cdots \\ \langle \phi_2 , A\phi_1 \rangle & \langle \phi_2 , A\phi_2 \rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Since
$$b_m = \sum_n A_{mn} a_n$$

In matrix notation

$$b = Aa$$

or
$$\begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

The transpose of A_{mn} is A^+

$$A^+_{mn} = A_{nm}$$

The adjoint A^+ of A is defined by

$$A^+_{mn} = (\phi_m , A^+ \phi_n) \neq$$

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$$A^+_{mn} = (A\phi_m, \phi_n) = (\phi_n, A\phi_m)^*$$

$$= A^*_{nm}$$

If A is Hermitian, $A^+ = A$, then

$$\boxed{A_{mn} = A^*_{nm} = A^+_{mn}}$$

<u>Some Identities:</u>

$$(AB)^+ = B^+ A^+$$

$$\det A^+ = \det A$$

$$\det(AB) = \det A \cdot \det B$$

$$(AB)^* = A^* B^*$$

$$\det A^* = (\det A)^*$$

$$\det A^+ = (\det A)^+$$

Some Properties :-

Real : $A = A^*$, $A_{mn} = A^*_{mn}$

Imaginary: $A = -A^*$, $A_{mn} = -A^*_{mn}$

Symmetric: $A = A^T$, $A_{mn} = A_{nm}$

Anti-symmetric: $A = -A^T$, $A_{mn} = -A_{nm}$
↓
skew

Hermitian : $A = A^\dagger$, $A_{mn} = A_{nm}$

Anti-Hermitian: $A = -A^\dagger$, $A_{mn} = -A_{nm}$

Orthogonal: $A^T = A^{-1}$, $AA^T = I$

Unitary: $A^\dagger = A^{-1}$, $AA^\dagger = I$

diagonal: $A_{mn} = A_{mm}\,\delta_{mn}$

Theorem: Prove that $\sum_p A_{mp} \cdot B_{pn} = (AB)_{mn}$

The product of two matrix representations is given by

$$\sum_p A_{mp} \cdot B_{pn} = \sum_p (\phi_m, A\phi_p)(\phi_p, B\phi_n)$$

$$= \sum_p \int \phi_m^* A \phi_p \, dx \int \phi_p^* B \phi_n \, dx'$$

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From the closure relation

$$\sum_p \phi_p^*(x) \phi_p(x') = \delta(x-x')$$

$$\sum_p A_{mp} B_{pn} = \iint \phi_m^* A \, \delta(x-x') \, B \phi_n \, dx$$

$$\int \delta(x-x') dx' = 1$$

$$= \int \phi_m^* A B \phi_n dx$$

$$\boxed{\sum_p A_{mp} B_{pn} = (AB)_{mn}} \text{ Proved.}$$

Eigenvalue Problem:

Consider the eigenvalue problem

$$A \phi_n = \lambda_n \phi_n$$

with $(\phi_m, \phi_n) = \delta_{mn}$. In the basis $\{\phi_n\}$ the matrix A is diagonal, with the diagonal elements as the eigen-values.

$$A_{mn} = (\phi_m, A\phi_n) = \lambda_n (\phi_m, \phi_n)$$

$$= \lambda_n \delta_{mn}$$

$$A = \begin{pmatrix} A_{11} & & 0 \\ & A_{22} & \\ 0 & & A_{33} \\ & & & \ddots \end{pmatrix} = \begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & 0 \\ 0 & & \lambda_3 \\ & & & \ddots \end{pmatrix}$$

The matrix of an operator in a basis of the eigenfunctions of that operator is diagonal.

Q. <u>The matrix representation of eigenfunctions ϕ_n (basis).</u>

The column vector representation of the eigenfunctions ϕ_n (basis) are the co-efficients $\{a_m^{(n)}\}$ in the expansion

$$\phi_n = \sum_m a_m^{(n)} \phi_m$$

Multiplying both sides by ϕ_p^* from the left and integrating over all space

$$\int \phi_p^* \phi_n \, dx = \sum_m a_m^{(n)} \int \phi_p^* \phi_m \, dx$$

$$\delta_{pn} = \sum_m a_m^{(n)} \delta_{pm}$$

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$$S_{pn} = a_p^{(n)}$$

$\Rightarrow$

$$\phi_1 \longrightarrow \begin{pmatrix} a_1^{(1)} \\ a_2^{(1)} \\ a_3^{(1)} \\ \vdots \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} - \text{for } n=$$

$$\phi_2 \longrightarrow \begin{pmatrix} a_1^{(2)} \\ a_2^{(2)} \\ a_3^{(2)} \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} - \text{for } n=$$

$$\phi_3 \longrightarrow \begin{pmatrix} a_1^{(3)} \\ a_2^{(3)} \\ a_3^{(3)} \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix} - \text{for } n=$$

Q The Eigenvalue Equation in the for[m] of Matrix Representation:

The eigenvalue equation can be writte[n] as

$$\hat{A}\phi_n = \lambda_n \phi_n$$

we know

$$\phi_n = \sum_m a_m^{(n)} \phi_m$$

or. $\langle \phi_n, \hat{A}\hat{I}\psi \rangle = \lambda \langle \phi_n, \hat{1}\psi \rangle$ (2-8)

$$\sum_m \langle \phi_n, A\phi_m \rangle \langle \underbrace{\phi_m, \psi}_{a_m} \rangle = \lambda \sum_m \underbrace{\langle \phi_n, \phi_m \rangle}_{\delta_{nm}} \langle \underbrace{\phi_m, \psi}_{a_m} \rangle$$

$$1 = \sum_m$$

$$\sum_m (A_{nm} - \lambda \delta_{nm}) a_m = 0$$

or

$$\begin{pmatrix} A_{11}-\lambda & A_{12} & A_{13} \cdots \\ A_{21} & A_{22}-\lambda & A_{23} \cdots \\ A_{31} & A_{32} & A_{33}-\lambda \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = 0$$

For the non-trivial Sol.

$$D(\lambda) = \det(A_{nm} - \lambda \delta_{nm}) = 0$$

This is known as the characteristic of Secular equation.

then

$$\sum_m A a_m^{(n)} \phi_m = \sum_m a_m^{(n)} \lambda_n \phi_m$$

multiplying both side by ϕ_p^* and integrated over all space.

$$\sum_m \int \phi_p^* A \phi_m \, dx \; a_m^{(n)} = \sum_m a_m^{(n)} \lambda_n \int \phi_p^* \phi_m \, dx$$

$$\sum_m a_m^{(n)} \int \phi_p^* A \phi_m \, dx = \lambda_n \sum_m a_m^{(n)} \delta_{pm}$$

$$\sum_m a_m^{(n)} (\phi_p, A\phi_m) = \lambda_n \sum_m a_m^{(n)} \delta_{pm}$$

$$\sum_m a_m^{(n)} A_{pm} = \lambda_n a_p^{(n)}$$

for $a^{(3)}$ the eigenvalue equation is

$\underline{\underline{n = 3.}}$

$$\begin{pmatrix} \cancel{\lambda_1} A_{11} & & 0 \\ & \cancel{\lambda_2} A_{22} & \\ 0 & & \cancel{A}_{33} \ddots \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \lambda_3 \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

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For $a^{(4)}$, $n=4$.

$$\begin{pmatrix} A_{11} & & & & \\ & A_{22} & & 0 & \\ & & A_{33} & & \\ & 0 & & A_{44} & \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} = \lambda_4 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$$

The Secular Equation:

Let us consider the eigenvalue probl

$$A\psi = \lambda\psi$$

ψ is an eigenfunction of A with eigenvalue λ. Let us work in the basis $\{\phi_n\}$

$$\langle \phi_n, \phi_m \rangle = \delta_{nm}$$

$$\psi = \sum_n a_n |\phi_n\rangle$$

with $a_n = \langle \phi_n, \psi \rangle$

From the eigenvalue equation, we

$$\langle \phi_n, A \cancel{\phi_n} \rangle = \lambda \langle \phi_n, \cancel{\phi_n} \rangle$$
$$\psi \qquad\qquad\qquad \psi$$

Unitary operator — Matrix Element

If the Hermitian adjoint U^{+} of an operator is equal to U^{-1} i.e.

$$U^{+} = U^{-1}$$

then U is said to be unitary.

The matrix elements of U satisfy

$$(U^{+})_{nm} = U^{-1}$$

$$(U_{mn})^{*} = (U^{-1})_{nm}.$$

$$(U^{T})^{*} = U^{-1}$$

$$UU^{+} = \hat{I}$$

$$(UU^{+})_{nm} = \delta_{nm}$$

$$\sum_{p} U_{np} \cdot (U_{mp})^{*} = \delta_{nm}$$

Since $(AB)_{nm} = \sum_{p} A \; B$

Traces:

The trace of a matrix A is the sum over its diagonal entries

$$\mathrm{Tr}\,\hat{A} = \sum_{q} A_{qq}$$

$$\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$$

$$\mathrm{Tr}(ABCD) = \mathrm{Tr}(BCDA) = \mathrm{Tr}(CDAB)$$

$$\mathrm{Tr}(A+B) = \mathrm{Tr}\,A + \mathrm{Tr}\,B$$

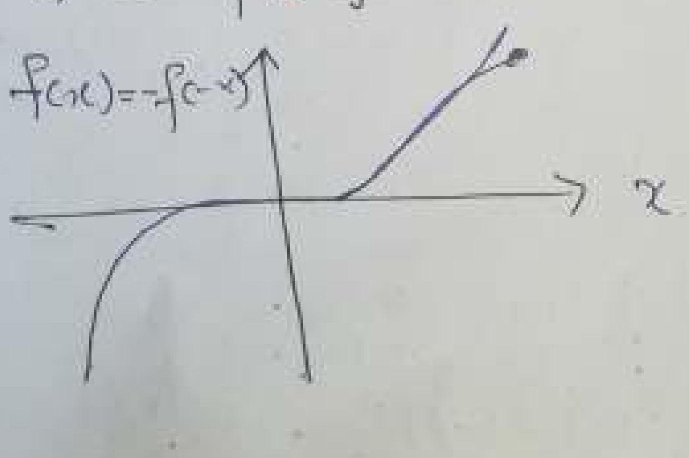
$$\mathrm{Tr}(AB-BA) = \mathrm{Tr}[A,B] = 0$$

$$\mathrm{Tr}\,A = \mathrm{Tr}(UAU^{-1}).$$

Parity operator:

A function has odd parity if

$$f(-x) = -f(x)$$



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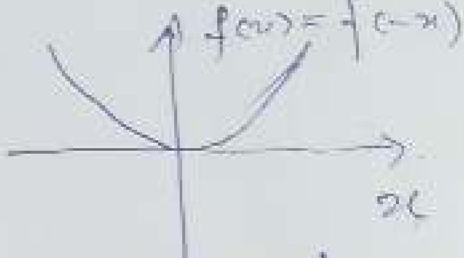
A function has even parity if

$f(x) = f(-x)$



A parity operator P is defined as

$$\hat{P} f(x) = f(-x)$$

Let us look at the eigenvalue of operator $\hat{P}$. Let "α" be the eigenvalue of $\hat{P}$

$$\hat{P} f(x) = f(-x) = \alpha f(x)$$

$$\hat{P}\hat{P} f(x) = \hat{P} f(-x) = f(x) = \alpha^2 f(x)$$

$\Rightarrow$

$$\alpha^2 = 1 \quad \text{or} \quad \alpha = \pm 1$$

for $\alpha = +1$, we optained

$$f(-x) = f(x) \quad \text{even parity}$$

for $\alpha = -1$

$$f(-x) = -f(x) \quad \text{odd parity}$$

Example: 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.11, 2.12, 2.13, 2.15, 2.19, 2.20

Solved Prob: 2.1, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 2.10, 2.11, 2.12, 2.13, 2.14, 2.16

Exercise: 2.1 – 2.6/, 2.16, 2.18, 2.25, 2.29 – 2.34