Chapter 13

Matrix Representation

Matrix Rep. → **Same basics as introduced already.**
Convenient method of working with vectors.

Superposition → **Complete set of vectors can be used to express any other vector.**

Complete set of N orthonormal vectors can form other complete sets of N orthonormal vectors.

Can find set of vectors for Hermitian operator satisfying

$$\underline{A}\left|u\right\rangle = \alpha\left|u\right\rangle.$$

Eigenvectors and eigenvalues

Matrix method → **Find superposition of basis states that are eigenstates of particular operator. Get eigenvalues.**

Orthonormal basis set in N dimensional vector space

$$\left\{ \left| e^j \right\rangle \right\}$$ **basis vectors**

Any N dimensional vector can be written as

$$\left| x \right\rangle = \sum_{j=1}^{N} x_j \left| e^j \right\rangle \qquad \text{with} \qquad x_j = \left\langle e^j \middle| x \right\rangle$$

To get this, project out

$\left| e^j \right\rangle \left\langle e^j \right|$ **from** $\left| x \right\rangle$

$x_j \left| e^j \right\rangle = \left| e^j \right\rangle \left\langle e^j \middle| x \right\rangle$ **piece of** $\left| x \right\rangle$ **that is** $\left| e^j \right\rangle$,

then sum over all $\left| e^j \right\rangle$.

Operator equation

$$\left| y \right\rangle = \underline{A} \left| x \right\rangle$$

$$\sum_{j=1}^{N} y_j \left| e^j \right\rangle = \underline{A} \sum_{j=1}^{N} x_j \left| e^j \right\rangle$$

Substituting the series in terms of bases vectors.

$$= \sum_{j=1}^{N} x_j \underline{A} \left| e^j \right\rangle$$

Left mult. by $\left\langle e^i \right|$

$$y_i = \sum_{j=1}^{N} \left\langle e^i \left| \underline{A} \right| e^j \right\rangle x_j$$

The N^2 scalar products

$$\left\langle e^i \left| \underline{A} \right| e^j \right\rangle$$

N values of j for each y_i; and N different y_i

are completely determined by

$\underline{A}$ and the basis set $\left\{ \left| e^j \right\rangle \right\}$.

Writing

$$a_{ij} = \langle e^i | \underline{A} | e^j \rangle$$

Matrix elements of $\underline{A}$ in the basis $\{|e^j\rangle\}$

gives for the linear transformation

$$y_i = \sum_{j=1}^{N} a_{ij} x_j \qquad j = 1, 2, \cdots N$$

Know the a_{ij} because we know $\underline{A}$ and $\{|e^j\rangle\}$

In terms of the vector representatives

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

$$\vec{Q} = 7\hat{x} + 5\hat{y} + 4\hat{z}$$ **vector**

$$\begin{bmatrix} 7 \\ 5 \\ 4 \end{bmatrix}$$ **vector representative, must know basis**

(Set of numbers, gives you vector when basis is known.)

The set of *N* linear algebraic equations can be written as

$$y = \underline{\underline{A}}\, x$$

double underline means matrix

$\underline{\underline{A}}$ array of coefficients - matrix

$$\underline{\underline{A}} = \left(a_{ij}\right) = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \vdots & & & \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix}$$

The a_{ij} are the elements of the matrix $\underline{\underline{A}}$.

$$y = \underline{\underline{A}}\,x$$

vector representatives in particular basis

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & & \\ \vdots & & & \vdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

The product of matrix $\underline{\underline{A}}$ and vector representative x is a new vector representative y with components

$$y_i = \sum_{j=1}^{N} a_{ij}\, x_j$$

Matrix Properties, Definitions, and Rules

Two matrices, $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are equal

$$\underline{\underline{A}} = \underline{\underline{B}}$$

if $a_{ij} = b_{ij}$.

The unit matrix

$$\underline{\underline{1}} = \underline{\underline{\delta}}_{ij} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

ones down principal diagonal

Gives identity transformation

$$y_i = \sum_{j=1}^{N} \delta_{ij} x_j = x_i$$

Corresponds to

$$|y\rangle = \underline{1}|x\rangle = |x\rangle$$

The zero matrix

$$\underline{\underline{0}} = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

$$\underline{\underline{0}}x = 0$$

Matrix multiplication

Consider

$$|y\rangle = \underline{A}|x\rangle \qquad |z\rangle = \underline{B}|y\rangle$$

operator equations

$$|z\rangle = \underline{B}\,\underline{A}|x\rangle$$

Using the same basis for both transformations

$$z_k = \sum_{i=1}^{N} b_{ki} y_i \qquad z = \underline{\underline{B}}\, y \qquad \underline{\underline{B}} = \text{ matrix } = (b_{ki})$$

$$z = \underline{\underline{B}} y = \underline{\underline{B}}\,\underline{\underline{A}}\, x = \underline{\underline{C}}\, x$$

$$\underline{\underline{C}} = \underline{\underline{B}}\,\underline{\underline{A}}$$

has elements

$$c_{kj} = \sum_{i=1}^{N} b_{ki} a_{ij}$$

Law of matrix multiplication

Example

$$\begin{pmatrix} 2 & 3 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} 7 & 5 \\ 5 & 6 \end{pmatrix} = \begin{pmatrix} 29 & 28 \\ 41 & 39 \end{pmatrix}$$

Multiplication Associative

$$\left(\underline{\underline{A}}\,\underline{\underline{B}}\right)\underline{\underline{C}} = \underline{\underline{A}}\left(\underline{\underline{B}}\,\underline{\underline{C}}\right)$$

Multiplication <u>NOT</u> Commutative except in special cases.

$$\underline{\underline{A}}\,\underline{\underline{B}} \neq \underline{\underline{B}}\,\underline{\underline{A}}$$

Matrix addition and multiplication by complex number

$$\alpha\,\underline{\underline{A}} + \beta\,\underline{\underline{B}} = \underline{\underline{C}}$$

$$c_{ij} = \alpha\, a_{ij} + \beta\, b_{ij}$$

Reciprocal of Product

$$\left(\underline{\underline{A}}\,\underline{\underline{B}}\right)^{-1} = \underline{\underline{B}}^{-1}\underline{\underline{A}}^{-1}$$

For matrix defined as $\underline{\underline{A}} = (a_{ij})$

Transpose

$$\tilde{\underline{\underline{A}}} = \left(a_{ji}\right)$$ **interchange rows and columns**

Complex Conjugate

$$\underline{\underline{A}}^{*} = \left(a_{ij}^{*}\right)$$ **complex conjugate of each element**

Hermitian Conjugate

$$\underline{\underline{A}}^{+} = \left(a_{ji}^{*}\right)$$ **complex conjugate transpose**

Inverse of a matrix $\underline{\underline{A}}$

inverse of $\underline{\underline{A}} \longrightarrow \underline{\underline{A}}^{-1}$

$$\underline{\underline{A}}\,\underline{\underline{A}}^{-1} = \underline{\underline{A}}^{-1}\underline{\underline{A}} = \underline{\underline{1}}$$ **identity matrix**

$$\underline{\underline{A}}^{-1} = \frac{\underline{\underline{A}}^{CT}}{\left|\underline{\underline{A}}\right|}$$

transpose of cofactor matrix (matrix of signed minors)

determinant

$\left|\underline{\underline{A}}\right| \neq 0$ **If** $\left|\underline{\underline{A}}\right| = 0$ $\underline{\underline{A}}$ **is singular**

Rules

$$\widetilde{(\underline{\underline{A}}\,\underline{\underline{B}})} = \tilde{\underline{\underline{B}}}\,\tilde{\underline{\underline{A}}}$$

transpose of product is product of transposes in reverse order

$$|\tilde{\underline{\underline{A}}}| = |\underline{\underline{A}}|$$

determinant of transpose is determinant

$$(\underline{\underline{A}}\,\underline{\underline{B}})^* = \underline{\underline{A}}^*\,\underline{\underline{B}}^*$$

complex conjugate of product is product of complex conjugates

$$|\underline{\underline{A}}^*| = |\underline{\underline{A}}|^*$$

determinant of complex conjugate is complex conjugate of determinant

$$(\underline{\underline{A}}\,\underline{\underline{B}})^+ = \underline{\underline{B}}^+\,\underline{\underline{A}}^+$$

Hermitian conjugate of product is product of Hermitian conjugates in reverse order

$$|\underline{\underline{A}}^+| = |\underline{\underline{A}}|^*$$

determinant of Hermitian conjugate is complex conjugate of determinant

Definitions

$\underline{\underline{A}} = \underline{\underline{\tilde{A}}}$ **Symmetric**

$\underline{\underline{A}} = \underline{\underline{A}}^{+}$ **Hermitian**

$\underline{\underline{A}} = \underline{\underline{A}}^{*}$ **Real**

$\underline{\underline{A}} = -\underline{\underline{A}}^{*}$ **Imaginary**

$\underline{\underline{A}}^{-1} = \underline{\underline{A}}^{+}$ **Unitary**

$a_{ij} = a_{ij}\,\delta_{ij}$ **Diagonal**

Powers of a matrix

$$\underline{\underline{A}}^{0} = \underline{\underline{1}} \qquad \underline{\underline{A}}^{1} = \underline{\underline{A}} \qquad \underline{\underline{A}}^{2} = \underline{\underline{A}}\,\underline{\underline{A}} \cdots$$

$$e^{\underline{\underline{A}}} = \underline{\underline{1}} + \underline{\underline{A}} + \frac{\underline{\underline{A}}^{2}}{2!} + \cdots$$

Column vector representative $\longrightarrow$ one column matrix

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

vector representatives in particular basis

then

$$y = \underline{\underline{A}}\, x$$

becomes

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & & \\ \vdots & & & \vdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

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row vector $\longrightarrow$ transpose of column vector

$$\tilde{x} = \left(x_1, x_2 \cdots x_N \right)$$

$$y = \underline{\underline{A}}\, x \longrightarrow \tilde{y} = \tilde{x}\, \tilde{\underline{\underline{A}}}$$ transpose

$$y = \underline{\underline{A}}\, x \longrightarrow y^{+} = x^{+}\, \underline{\underline{A}}^{+}$$ Hermitian conjugate

Change of Basis

orthonormal basis

$$\left\{ \left| e^i \right\rangle \right\}$$

then

$$\left\langle e^i \middle| e^j \right\rangle = \delta_{ij} \qquad \left(i, j = 1, 2, \cdots N \right)$$

Superposition of $\left\{ \left| e^i \right\rangle \right\}$ $\Longrightarrow$ **can form *N* new vectors linearly independent**

a new basis $\left\{ \left| e^{i'} \right\rangle \right\}$

$$\left| e^{i'} \right\rangle = \sum_{k=1}^{N} u_{ik} \left| e^k \right\rangle \qquad i = 1,\ 2, \quad \cdots \quad N$$

complex numbers

New Basis is Orthonormal

$$\langle e^{j'} | e^{i'} \rangle = \delta_{ij}$$

if the matrix

$$\underline{\underline{U}} = (u_{ik})$$

coefficients in superposition

$$|e^{i'}\rangle = \sum_{k=1}^{N} u_{ik} |e^{k}\rangle \qquad i = 1,\ 2, \quad \cdots \quad N$$

meets the condition

$$\underline{\underline{U}}^{+} \underline{\underline{U}} = \underline{\underline{1}}$$

$$\Rightarrow \quad \underline{\underline{U}}^{-1} = \underline{\underline{U}}^{+}$$

$\underline{\underline{U}}$ **is unitary – Hermitian conjugate = inverse**

Important result. The new basis $\{|e^{i'}\rangle\}$ will be orthonormal if $\underline{\underline{U}}$, the transformation matrix, is unitary (see book and Errata and Addenda, linear algebra book).

$$\underline{\underline{U}}\,\underline{\underline{U}}^{+} = \underline{\underline{U}}^{+} \underline{\underline{U}} = \underline{\underline{1}}$$

Unitary transformation
substitutes orthonormal basis $\{|e'\rangle\}$ for orthonormal basis $\{|e\rangle\}$.

Vector $|x\rangle$

$$|x\rangle = \sum_i x_i |e^i\rangle$$

$$|x\rangle = \sum_i x'_i |e^{i'}\rangle$$

vector – line in space (may be high dimensionality abstract space)
written in terms of two basis sets

$|x\rangle$ Same vector – different basis.

The unitary transformation $\underline{\underline{U}}$ can be used to change a vector representative of $|x\rangle$ in one orthonormal basis set to its vector representative in another orthonormal basis set.

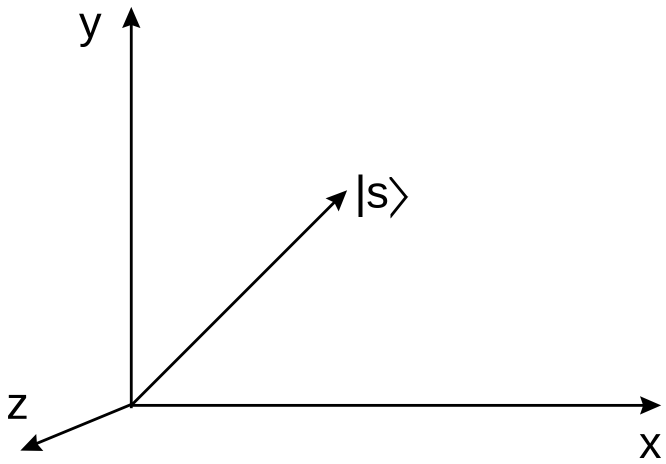
x – vector rep. in unprimed basis
x' – vector rep. in primed basis

$x' = \underline{\underline{U}}\, x$ **change from unprimed to primed basis**

$x = \underline{\underline{U}}^{+}\, x'$ **change from primed to unprimed basis**

Example

Consider basis $\{\hat{x}, \hat{y}, \hat{z}\}$



Vector $|s\rangle$ **- line in real space.**

In terms of basis $|s\rangle = 7\hat{x} + 7\hat{y} + 1\hat{z}$

Vector representative in basis $\{\hat{x}, \hat{y}, \hat{z}\}$

$$s = \begin{bmatrix} 7 \\ 7 \\ 1 \end{bmatrix}$$

Change basis by rotating axis system 45° around $\hat{z}$.

Can find the new representative of $|s\rangle$, s'

$$s' = \underline{\underline{U}}\, s$$

$\underline{\underline{U}}$ **is rotation matrix**

$$\underline{\underline{U}} = \begin{array}{c} \begin{array}{ccc} \quad x & \qquad\qquad y & \qquad z \end{array} \\ \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{array}$$

For 45° rotation around z

$$\underline{\underline{U}} = \begin{pmatrix} \sqrt{2}/2 & \sqrt{2}/2 & 0 \\ -\sqrt{2}/2 & \sqrt{2}/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Then

$$s' = \begin{pmatrix} \sqrt{2}/2 & \sqrt{2}/2 & 0 \\ -\sqrt{2}/2 & \sqrt{2}/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 7 \\ 7 \\ 1 \end{pmatrix} = \begin{pmatrix} 7\sqrt{2} \\ 0 \\ 1 \end{pmatrix}$$

$$s' = \begin{bmatrix} 7\sqrt{2} \\ 0 \\ 1 \end{bmatrix}$$ vector representative of $|s\rangle$ in basis $\{|e'\rangle\}$

Same vector but in new basis.
Properties unchanged.

Example – length of vector $\left(\langle s|s\rangle\right)^{1/2}$

$$\left[\langle s|s\rangle\right]^{1/2} = (s^{*}\cdot s)^{1/2} = (49+49+1)^{1/2} = (99)^{1/2}$$

$$\left[\langle s|s\rangle\right]^{1/2} = (s'^{*}\cdot s')^{1/2} = (2\times 49+0+1)^{1/2} = (99)^{1/2}$$

Can go back and forth between representatives of a vector $|x\rangle$ by

change from unprimed to primed basis

$$\boldsymbol{x}' = \underline{\underline{U}}\,\boldsymbol{x}$$

change from primed to unprimed basis

$$\boldsymbol{x} = \underline{\underline{U}}^{+}\,\boldsymbol{x}'$$

components of $|x\rangle$ in different basis

Consider the linear transformation

$$|y\rangle = \underline{A}|x\rangle$$ operator equation

In the basis $\{|e\rangle\}$ can write

$$y = \underline{\underline{A}}\, x$$

or

$$y_i = \sum_j a_{ij} x_j$$

Change to new orthonormal basis $\{|e'\rangle\}$ using $\underline{\underline{U}}$

$$y' = \underline{\underline{U}}\, y = \underline{\underline{U}}\,\underline{\underline{A}}\, x = \underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{+} x'$$

or

$$y' = \underline{\underline{A}}' x'$$

with the matrix $\underline{\underline{A}}'$ given by

$$\underline{\underline{A}}' = \underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{+}$$

Because $\underline{\underline{U}}$ is unitary $$\underline{\underline{A}}' = \underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{-1}$$

Extremely Important

$$\underline{\underline{A}}' = \underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{-1}$$

Can change the matrix representing an operator in one orthonormal basis into the equivalent matrix in a different orthonormal basis.

Called

Similarity Transformation

$$y = \underline{\underline{A}}\, x \qquad \underline{\underline{A}}\,\underline{\underline{B}} = \underline{\underline{C}} \qquad \underline{\underline{A}} + \underline{\underline{B}} = \underline{\underline{C}}$$

In basis $\{|e\rangle\}$

Go into basis $\{|e'\rangle\}$

$$y' = \underline{\underline{A}}'\, x' \qquad \underline{\underline{A}}'\,\underline{\underline{B}}' = \underline{\underline{C}}' \qquad \underline{\underline{A}}' + \underline{\underline{B}}' = \underline{\underline{C}}'$$

Relations unchanged by change of basis.

Example $\underline{\underline{A}}\,\underline{\underline{B}} = \underline{\underline{C}}$

$$\underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{B}}\,\underline{\underline{U}}^{+} = \underline{\underline{U}}\,\underline{\underline{C}}\,\underline{\underline{U}}^{+}$$

Can insert $\underline{\underline{U}}^{+}\underline{\underline{U}}$ **between** $\underline{\underline{A}}\,\underline{\underline{B}}$ **because** $\underline{\underline{U}}^{+}\underline{\underline{U}} = \underline{\underline{U}}^{-1}\underline{\underline{U}} = \underline{\underline{1}}$

$$\underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{+}\underline{\underline{U}}\,\underline{\underline{B}}\,\underline{\underline{U}}^{+} = \underline{\underline{U}}\,\underline{\underline{C}}\,\underline{\underline{U}}^{+}$$

Therefore

$$\underline{\underline{A}}'\,\underline{\underline{B}}' = \underline{\underline{C}}'$$

Isomorphism between operators in abstract vector space and matrix representatives.

Because of isomorphism not necessary to distinguish abstract vectors and operators from their matrix representatives.

The matrices (for operators) and the representatives (for vectors) can be used in place of the real things.

Hermitian Operators and Matrices

Hermitian operator

$$\langle x | \underline{A} | y \rangle = \overline{\langle y | \underline{A} | x \rangle}$$

Hermitian operator $\longrightarrow$ Hermitian Matrix

$$\underline{\underline{A}} = \underline{\underline{A}}^{+}$$

+ - complex conjugate transpose - Hermitian conjugate

Theorem (Proof: Powell and Craseman, P. 303 – 307, or linear algebra book)

For a Hermitian operator $\underline{A}$ in a linear vector space of N dimensions,

there exists an orthonormal basis,

$$\left|U^1\right\rangle, \left|U^2\right\rangle \cdots \left|U^N\right\rangle$$

relative to which $\underline{A}$ is represented by a diagonal matrix

$$\underline{\underline{A}}' = \begin{pmatrix} \alpha_1 & 0 & 0 & \cdots \\ 0 & \alpha_2 & & 0 \\ 0 & & & \vdots \\ \vdots & 0 & \cdots & \alpha_N \end{pmatrix} .$$

The vectors, $\left|U^i\right\rangle$, and the corresponding real numbers, α_i, are the solutions of the Eigenvalue Equation

$$\underline{A}\left|U\right\rangle = \alpha\left|U\right\rangle$$

and there are no others.

Application of Theorem

Operator $\underline{A}$ represented by matrix $\underline{\underline{A}}$

in some basis $\left\{\left|e^i\right\rangle\right\}$. The basis is any convenient basis.

In general, the matrix will not be diagonal.

There exists some new basis $\longrightarrow$ eigenvectors

$\left\{\left|U^i\right\rangle\right\}$

in which $\underline{\underline{A}}'$ represents operator and is diagonal $\longrightarrow$ eigenvalues.

To get from $\left\{\left|e^i\right\rangle\right\}$ to $\left\{\left|U^i\right\rangle\right\}$

$\longrightarrow$ unitary transformation.

$$\left\{\left|U^i\right\rangle\right\} = \underline{\underline{U}}\left\{\left|e^i\right\rangle\right\}.$$

$$\underline{\underline{A}}' = \underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{-1}$$

Similarity transformation takes matrix in arbitrary basis into diagonal matrix with eigenvalues on the diagonal.

Matrices and Q.M.

Previously represented state of system by vector $\left|\ \right\rangle$ in abstract vector space.

Dynamical variables represented by linear operators.

Operators produce linear transformations. $\left|y\right\rangle = \underline{A}\left|x\right\rangle$

Real dynamical variables (observables) are represented by Hermitian operators.

Observables are eigenvalues of Hermitian operators. $\underline{A}\left|S\right\rangle = \alpha\left|S\right\rangle$

Solution of eigenvalue problem gives eigenvalues and eigenvectors.

Matrix Representation

Hermitian operators replaced by Hermitian matrix representations.

$$\underline{A} \rightarrow \underline{\underline{A}}$$

In proper basis, $\underline{\underline{A}}'$ is the diagonal Hermitian matrix and the diagonal matrix elements are the eigenvalues (observables).

A suitable transformation $\underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{-1}$ takes $\underline{\underline{A}}$ (arbitrary basis) into $\underline{\underline{A}}'$ (diagonal – eigenvector basis)

$$\underline{\underline{A}}' = \underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{-1}.$$

$\underline{\underline{U}}$ **takes arbitrary basis into eigenvectors.**

Diagonalization of matrix gives eigenvalues and eigenvectors.

Matrix formulation is another way of dealing with operators and solving eigenvalue problems.

All rules about kets, operators, etc. still apply.

Example

Two Hermitian matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$

can be simultaneously diagonalized by the same unitary transformation if and only if they commute.

All ideas about matrices also true for infinite dimensional matrices.

Example – Harmonic Oscillator

Have already solved – use occupation number representation kets and bras (already diagonal).

$$\underline{H} = \frac{1}{2}\left(\underline{P}^2 + \underline{x}^2\right) = \frac{1}{2}\left(\underline{a}\,\underline{a}^+ + \underline{a}^+\underline{a}\right)$$

$$\underline{a}|n\rangle = \sqrt{n}\,|n-1\rangle \qquad \underline{a}^+|n\rangle = \sqrt{n+1}\;|n+1\rangle$$

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matrix elements of $\underline{a}$

$$\langle 0|\underline{a}|0\rangle = 0$$
$$\langle 0|\underline{a}|1\rangle = \sqrt{1}$$
$$\langle 0|\underline{a}|2\rangle = 0$$
$$\vdots$$
$$\langle 1|\underline{a}|0\rangle = 0$$
$$\langle 1|\underline{a}|1\rangle = 0$$
$$\langle 1|\underline{a}|2\rangle = \sqrt{2}$$
$$\langle 1|\underline{a}|3\rangle = 0$$
$$\vdots$$

$$\underline{\underline{a}} = \begin{array}{c c} & \begin{array}{cccccccc} |0\rangle & |1\rangle & |2\rangle & |3\rangle & \cdot & \cdot & \cdot & \cdot \end{array} \\ \begin{array}{c} \langle 0| \\ \langle 1| \\ \langle 2| \\ \langle 3| \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{array} & \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & \sqrt{2} & 0 & 0 & & & \\ 0 & 0 & 0 & \sqrt{3} & 0 & & & \\ 0 & 0 & 0 & 0 & \sqrt{4} & & & \\ \cdot & & & & & \cdot & & \\ \cdot & & & & & & \cdot & \\ \cdot & & & & & & & \cdot \\ \cdot & & & & & & & \end{pmatrix} \end{array}$$

$$\underline{\underline{a}}^{+} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdot & \cdot \\ \sqrt{1} & 0 & 0 & 0 & \cdot & \cdot \\ 0 & \sqrt{2} & 0 & 0 & \cdot & \cdot \\ 0 & 0 & \sqrt{3} & 0 & \cdot & \cdot \\ 0 & 0 & 0 & \sqrt{4} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$\underline{\underline{H}} = \frac{1}{2}\left(\underline{\underline{a}}\,\underline{\underline{a}}^{+} + \underline{\underline{a}}^{+}\,\underline{\underline{a}}\right)$$

$$\underline{\underline{a}}\,\underline{\underline{a}}^{+} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdot & \cdot \\ 0 & 0 & \sqrt{2} & 0 & \cdot & \cdot \\ 0 & 0 & 0 & \sqrt{3} & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & \cdot & \cdot \\ \sqrt{1} & 0 & 0 & 0 & \cdot & \cdot \\ 0 & \sqrt{2} & 0 & 0 & \cdot & \cdot \\ 0 & 0 & \sqrt{3} & 0 & \cdot & \cdot \\ 0 & 0 & 0 & \sqrt{4} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdot \\ 0 & 2 & 0 & 0 & \cdot \\ 0 & 0 & 3 & 0 & \cdot \\ 0 & 0 & 0 & 4 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$\underline{\underline{H}} = \frac{1}{2}\left(\underline{\underline{a}}\,\underline{\underline{a}}^{+} + \underline{\underline{a}}^{+}\,\underline{\underline{a}}\right)$$

$$\underline{\underline{a}}^{+}\,\underline{\underline{a}} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot \\ \sqrt{1} & 0 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & \sqrt{2} & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & \sqrt{3} & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \sqrt{4} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdot & \cdot \\ 0 & 0 & \sqrt{2} & 0 & \cdot & \cdot \\ 0 & 0 & 0 & \sqrt{3} & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdot \\ 0 & 1 & 0 & 0 & \cdot \\ 0 & 0 & 2 & 0 & \cdot \\ 0 & 0 & 0 & 3 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Adding the matrices $\underline{\underline{a}}\,\underline{\underline{a}}^+$ and $\underline{\underline{a}}^+\underline{\underline{a}}$ and multiplying by ½ gives $\underline{\underline{H}}$

$$\underline{\underline{H}} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 & \cdot \\ 0 & 3 & 0 & 0 & \cdot \\ 0 & 0 & 5 & 0 & \cdot \\ 0 & 0 & 0 & 7 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} = \begin{pmatrix} 1/2 & 0 & 0 & 0 & \cdot \\ 0 & 3/2 & 0 & 0 & \cdot \\ 0 & 0 & 5/2 & 0 & \cdot \\ 0 & 0 & 0 & 7/2 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

The matrix is diagonal with eigenvalues on diagonal. In normal units the matrix would be multiplied by $\hbar\omega$.

This example shows idea, but not how to diagonalize matrix when you don't already know the eigenvectors.

Diagonalization

Eigenvalue equation

eigenvalue

$$\underline{\underline{A}}\,u = \alpha u \longrightarrow \underline{\underline{A}}\,u - \alpha u = 0$$

matrix representing operator

representative of eigenvector

In terms of the components

$$\sum_{j=1}^{N}\left(a_{ij} - \alpha\,\delta_{ij}\right)u_j = 0 \qquad \left(i = 1, 2 \cdots N\right)$$

This represents a system of equations

$$\left(a_{11} - \alpha\right)u_1 + a_{12}u_2 + a_{13}u_3 + \cdots \quad = 0$$

$$a_{21}u_1 + \left(a_{22} - \alpha\right)u_2 + a_{23}u_3 + \cdots \quad = 0$$

$$a_{31}u_1 + a_{32}u_2 + \left(a_{33} - \alpha\right)u_3 + \cdots \quad = 0$$

We know the a_{ij}.

We don't know

α - the eigenvalues

u_i - the vector representatives, one for each eigenvalue.

Besides the trivial solution

$$u_1 = u_2 = \cdots u_N = 0$$

A solution only exists if the determinant of the coefficients of the u_i vanishes.

$$\begin{vmatrix} (a_{11}-\alpha) & a_{12} & a_{13} & \cdot & \cdot & \cdot \\ a_{21} & (a_{22}-\alpha) & a_{23} & \cdot & \cdot & \cdot \\ a_{31} & a_{32} & (a_{33}-\alpha) & & & \\ \cdot & & & \cdot & & \\ \cdot & & & & \cdot & \\ \cdot & & & & & \cdot \end{vmatrix} = 0$$

know a_{ij}, don't know α's

Expanding the determinant gives N^{th} degree equation for the unknown α's (eigenvalues).

Then substituting one eigenvalue at a time into system of equations, the u_i (eigenvector representatives) are found.
N equations for u's gives only N - 1 conditions.

$$(a_{11}-\alpha)u_1 + a_{12}u_2 + a_{13}u_3 + \cdots \quad = 0$$

$$a_{21}u_1 + (a_{22}-\alpha)u_2 + a_{23}u_3 + \cdots \quad = 0$$

$$a_{31}u_1 + a_{32}u_2 + (a_{33}-\alpha)u_3 + \cdots \quad = 0$$

Use normalization.

$$u_1^* u_1 + u_2^* u_2 + \cdots + u_N^* u_N = 1$$

Example - Degenerate Two State Problem

Basis - time independent kets $|\alpha\rangle \quad |\beta\rangle$ **orthonormal.**

$$\underline{H}|\alpha\rangle = E_0|\alpha\rangle + \gamma|\beta\rangle$$

$$\underline{H}|\beta\rangle = E_0|\beta\rangle + \gamma|\alpha\rangle$$

α and β not eigenkets.
Coupling γ.

These equations define $\underline{H}$.

The matrix elements are

$$\langle\alpha|\underline{H}|\alpha\rangle = E_0$$
$$\langle\beta|\underline{H}|\alpha\rangle = \gamma$$
$$\langle\alpha|\underline{H}|\beta\rangle = \gamma$$
$$\langle\beta|\underline{H}|\beta\rangle = E_0$$

And the Hamiltonian matrix is

$$\underline{\underline{H}} = \begin{array}{c} \\ \langle\alpha| \\ \langle\beta| \end{array} \begin{array}{c} \begin{array}{cc} |\alpha\rangle & |\beta\rangle \end{array} \\ \begin{pmatrix} E_0 & \gamma \\ \gamma & E_0 \end{pmatrix} \end{array}$$

The corresponding system of equations is

$$(E_0 - \lambda)\left|\alpha\right\rangle + \gamma\left|\beta\right\rangle = 0$$

$$\gamma\left|\alpha\right\rangle + (E_0 - \lambda)\left|\beta\right\rangle = 0$$

These only have a solution if the determinant of the coefficients vanish.

$$\begin{vmatrix} E_0 - \lambda & \gamma \\ \gamma & E_0 - \lambda \end{vmatrix} = 0$$

Take the matrix $\begin{pmatrix} E_0 & \gamma \\ \gamma & E_0 \end{pmatrix}$

Make into determinant. Subtract λ from the diagonal elements.

Expanding

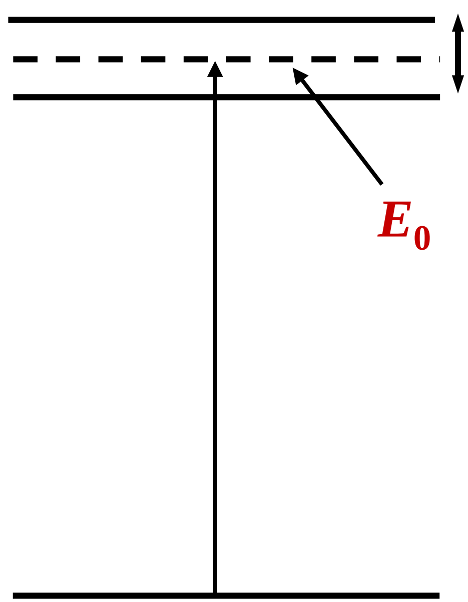
$$\left(E_0 - \lambda\right)^2 - \gamma^2 = 0$$

$$\lambda^2 - 2E_0\lambda + E_0^2 - \gamma^2 = 0$$

Energy Eigenvalues

$$\lambda_+ = E_0 + \gamma$$

$$\lambda_- = E_0 - \gamma$$



To obtain Eigenvectors

Use system of equations for each eigenvalue.

$$|+\rangle = a_+|\alpha\rangle + b_+|\beta\rangle$$

$$|-\rangle = a_-|\alpha\rangle + b_-|\beta\rangle$$

Eigenvectors associated with λ_+ and λ_-.

$[a_+, b_+]$ and $[a_-, b_-]$ are the vector representatives of $|+\rangle$ and $|-\rangle$ in the $|\alpha\rangle, |\beta\rangle$ basis set.

We want to find these.

First, for the

$$\lambda_+ = E_0 + \gamma \qquad \text{eigenvalue}$$

write system of equations.

$$(H_{11} - \lambda_+)a_+ + H_{12}b_+ = 0$$

$$H_{21}a_+ + (H_{22} - \lambda_+)b_+ = 0$$

$$H_{11} = H_{\alpha\alpha}; \quad H_{12} = H_{\alpha\beta}; \quad H_{21} = H_{\beta\alpha}; \quad H_{22} = H_{\beta\beta}$$

Matrix elements of $\underline{\underline{H}}$

$$(E_0 - E_0 - \gamma)a_+ + \gamma b_+ = 0$$

$$\gamma a_+ + (E_0 - E_0 - \gamma)b_+ = 0$$

The matrix elements are

$$\langle \alpha | \underline{H} | \alpha \rangle = E_0$$
$$\langle \beta | \underline{H} | \alpha \rangle = \gamma$$
$$\langle \alpha | \underline{H} | \beta \rangle = \gamma$$
$$\langle \beta | \underline{H} | \beta \rangle = E_0$$

The result is

$$-\gamma a_+ + \gamma b_+ = 0$$

$$\gamma a_+ - \gamma b_+ = 0$$

An equivalent way to get the equations is to use a matrix form.

$$\begin{pmatrix} E_0-\lambda_+ & \gamma \\ \gamma & E_0-\lambda_+ \end{pmatrix}\begin{pmatrix} a_+ \\ b_+ \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Substitute $\lambda_+ = E_0+\gamma$

$$\begin{pmatrix} E_0-E_0-\gamma & \gamma \\ \gamma & E_0-E_0-\gamma \end{pmatrix}\begin{pmatrix} a_+ \\ b_+ \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} -\gamma & \gamma \\ \gamma & -\gamma \end{pmatrix}\begin{pmatrix} a_+ \\ b_+ \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Multiplying the matrix by the column vector representative gives equations.

$$-\gamma a_+ + \gamma b_+ = 0$$

$$\gamma a_+ - \gamma b_+ = 0$$

$$-\gamma a_+ + \gamma b_+ = 0$$

The two equations are identical.

$$\gamma a_+ - \gamma b_+ = 0$$

$$a_+ = b_+$$

Always get *N* – 1 conditions for the *N* unknown components.
Normalization condition gives necessary additional equation.

$$a_+^2 + b_+^2 = 1$$

Then

$$a_+ = b_+ = \frac{1}{\sqrt{2}}$$

and

$$|+\rangle = \frac{1}{\sqrt{2}}|\alpha\rangle + \frac{1}{\sqrt{2}}|\beta\rangle$$

Eigenvector in terms of the $|\alpha\rangle$ $|\beta\rangle$ basis set.

For the eigenvalue

$$\lambda_- = E_0 - \gamma$$

using the matrix form to write out the equations

$$\begin{pmatrix} E_0 - \lambda_- & \gamma \\ \gamma & E_0 - \lambda_- \end{pmatrix}\begin{pmatrix} a_- \\ b_- \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Substituting $\lambda_- = E_0 - \gamma$

$$\begin{pmatrix} \gamma & \gamma \\ \gamma & \gamma \end{pmatrix}\begin{pmatrix} a_- \\ b_- \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\gamma a_- + \gamma b_- = 0$$

$$\gamma a_- + \gamma b_- = 0$$

These equations give $a_- = -b_-$

Using normalization $a_- = \dfrac{1}{\sqrt{2}}$ $\qquad b_- = -\dfrac{1}{\sqrt{2}}$

Therefore $\quad \left|-\right\rangle = \dfrac{1}{\sqrt{2}}\left|\alpha\right\rangle - \dfrac{1}{\sqrt{2}}\left|\beta\right\rangle$

Can diagonalize by transformation

$$\underline{\underline{H}}' = \underline{\underline{U}}\,\underline{\underline{H}}\,\underline{\underline{U}}^{-1}$$

diagonal   not diagonal

Transformation matrix consists of representatives of eigenvectors in original basis.

$$\underline{\underline{U}} = \begin{pmatrix} a_+ & a_- \\ b_+ & b_- \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$$

$$\underline{\underline{U}}^{-1} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$$

complex conjugate transpose

Then

$$\underline{\underline{H}}' = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \begin{pmatrix} E_0 & \gamma \\ \gamma & E_0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$$

Factoring out $1/\sqrt{2}$, one from each matrix.

$$\underline{\underline{H}}' = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} E_0 & \gamma \\ \gamma & E_0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

after matrix multiplication

$$\underline{\underline{H}}' = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} E_0 + \gamma & E_0 - \gamma \\ E_0 + \gamma & -E_0 + \gamma \end{pmatrix}$$

more matrix multiplication

$$\underline{\underline{H}}' = \begin{pmatrix} E_0 + \gamma & 0 \\ 0 & E_0 - \gamma \end{pmatrix}$$

diagonal with eigenvalues on diagonal