Chapter 4 Matrices, Eigenvalue problems

In this chapter, we discuss the matrices which is necessary for the discussion of quantum mechanics. The Mathematica programs for the matrices can be obtained from my web site (Lecture note on computational physics Phys.468).

http://bingweb.binghamton.edu/~suzuki/

4.1 Dirac Notation

The quantum state of any physical system is characterized by a state vector, belonging to a Hilbert space H which is the state space of the system.

Ket vector $|\psi\rangle$,

Bra vector: $\langle\psi|$,

which is associated with the ket $|\psi\rangle$

(1) Dual correspondence:

$$\lambda|\psi\rangle \overset{DC}{\longleftrightarrow} \lambda^*\langle\psi| \ (\lambda\text{: complex number}).$$

$\lambda^*\langle\psi|$ represents the bra vector associated with the ket vector $\lambda|\psi\rangle$.

$$|\alpha\rangle + |\beta\rangle \overset{DC}{\longleftrightarrow} \langle\alpha| + \langle\beta|,$$

$$C_\alpha|\alpha\rangle + C_\beta|\beta\rangle \overset{DC}{\longleftrightarrow} C_\alpha{}^*\langle\alpha| + C_\beta{}^*\langle\beta|.$$

(2) Inner product:

$$\langle\alpha|\beta\rangle = (\langle\alpha|)(|\beta\rangle).$$

The inner product is, in general, a complex number. The properties of the inner product is as follows.

1. $\langle\alpha|\beta\rangle^* = \langle\beta|\alpha\rangle$.

2. $\langle\alpha|\alpha\rangle^* = \langle\alpha|\alpha\rangle$. real positive number.

(3) Linear operator; $\hat{A}$ such as spin, momentum, coordinate,

If

$$|\psi> \in H \text{ and } |\psi'> \in H,$$

then we have

$$|\psi'\rangle = \hat{A}|\psi\rangle.$$

Note that

$$\hat{A}(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle) = \lambda_1\hat{A}|\psi_1\rangle + \lambda_2\hat{A}|\psi_2\rangle),$$

$$(\hat{A}\,\hat{B})|\psi\rangle = \hat{A}(\hat{B})|\psi\rangle.$$

(4) Commutation relation

In general, we have

$$\hat{A}\,\hat{B} \neq \hat{B}\,\hat{A}.$$

Commutator is defined as

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}.$$

((Example))

$$[\hat{x}, \hat{p}] = i\hbar.$$

(5) Outerproduct

The outer product of $|\beta\rangle$ and $\langle\alpha|$ is an operator, which is defined by

$$\hat{A} = |\beta\rangle\langle\alpha|.$$

Note that

$$\hat{A}|\psi\rangle = (|\beta\rangle\langle\alpha|)|\psi\rangle = \langle\alpha|\psi\rangle|\beta\rangle.$$

4.2 Hermitian conjugate

$\hat{A}^+$ is called an adjoint operator or Hermitian conjugate of $\hat{A}$.

$$|\psi\rangle \overset{\hat{A}}{\longleftrightarrow} |\psi'\rangle = \hat{A}|\psi\rangle .$$

Hermitian conjugate:

$$\langle\psi| \leftrightarrow \langle\psi'| = \langle\psi|\hat{A}^{+} .$$

Since $\langle\psi'|\varphi\rangle = \langle\varphi|\psi\rangle^{*}$, we have the following relation (in general valid)

$$\langle\psi|\hat{A}^{+}|\varphi\rangle = \langle\varphi|\hat{A}|\psi\rangle^{*}. \qquad (3)$$

(A) Correspondence between an operator and its adjoint

1. $(\hat{A}^{+})^{+} = \hat{A}$
2. $(\lambda\hat{A})^{+} = \lambda^{*}\hat{A}^{+}$
3. $(\hat{A}+\hat{B})^{+} = \hat{A}^{+} + \hat{B}^{+}$
4. $(\hat{A}\hat{B})^{+} = \hat{B}^{+}\hat{A}^{+}$

((Proof))
We have

$$\langle\psi|(\hat{A}\hat{B})^{+}|\varphi\rangle = \langle\varphi|(\hat{A}\hat{B})|\psi\rangle^{*} = \langle\alpha|\beta\rangle^{*} = \langle\beta|\alpha\rangle = \langle\psi|\hat{B}^{+}\hat{A}^{+}|\varphi\rangle ,$$

where

$$\langle\alpha| = \langle\varphi|\hat{A}, \quad \text{and} \quad |\beta\rangle = \hat{B}|\psi\rangle,$$

or

$$|\alpha\rangle = \hat{A}^{+}|\varphi\rangle, \quad \text{and} \quad \langle\beta| = \langle\psi|\hat{B}^{+} .$$

(B) Hermitian conjugate of $|\beta\rangle\langle\alpha|$

$$\hat{A} = |\beta\rangle\langle\alpha|, \qquad \hat{A}^{+} = |\alpha\rangle\langle\beta| .$$

((Proof))

$$\langle\gamma|\hat{A}^{+}|\delta\rangle = \langle\delta|\hat{A}|\gamma\rangle^{*} = (\langle\delta|\beta\rangle\langle\alpha|\gamma\rangle)^{*} = \langle\delta|\beta\rangle^{*}\langle\alpha|\gamma\rangle^{*} = \langle\beta|\delta\rangle\langle\gamma|\alpha\rangle = \langle\gamma|\alpha\rangle\langle\beta|\delta\rangle .$$

Thus we have

$$\hat{A}^{+} = |\alpha\rangle\langle\beta| .$$

(C) Hermitian conjugate of the complex number

$$\langle\psi|c|\varphi\rangle^{*} = \langle\varphi|c^{+}|\psi\rangle , \qquad (c\text{: complex number})$$

or

$$\langle\psi|c|\varphi\rangle^{*} = \left(c\langle\psi|\varphi\rangle\right)^{*} = c^{*}\langle\psi|\varphi\rangle^{*} = c^{*}\langle\varphi|\psi\rangle = \langle\varphi|c^{*}|\psi\rangle ,$$

where c is the complex number.

Then we have

$$\langle\varphi|c^{+}|\psi\rangle = \langle\varphi|c^{*}|\psi\rangle ,$$

or

$$c^{+} = c^{*} .$$

When $c = i$ (pure imaginary),

$$i^{+} = i^{*} = -i .$$

4.3 Definition of Hermitian operator

We start from the definition of Hermitian conjugate (or Hermitian adjoint)
Hermite conjugate (definition): or Hermitian adjoint

$$\langle\psi|\hat{O}|\varphi\rangle^{*} = \langle\varphi|\hat{O}^{+}|\psi\rangle . \qquad (1)$$

for any operator $\hat{O}$ and any $|\psi\rangle$ In quantum mechanics, the expectation value should be real, i.e.,

$$\langle\psi|\hat{A}|\psi\rangle^{*} = \langle\psi|\hat{A}|\psi\rangle . \qquad (2)$$

In Eq.(1) with $\hat{O} = \hat{A}$,

$$\langle \psi | \hat{A} | \psi \rangle^* = \langle \psi | \hat{A}^+ | \psi \rangle . \tag{3}$$

Then we have

$$\langle \psi | \hat{A} | \psi \rangle = \langle \psi | \hat{A}^+ | \psi \rangle ,$$

from Eqs.(2) and (3), leading to

$$\hat{A}^+ = \hat{A}.$$

This means that $\hat{A}$ is the Hermitian operator.

Suppose that $\hat{A}$ and $\hat{B}$ are Hermitian; $\hat{A}^+ = \hat{A}$ and $\hat{B}^+ = \hat{B}$. Then we have

1. $\left(\hat{A}\hat{B}\right)^+ = \hat{B}^+\hat{A}^+ = \hat{B}\hat{A}$, So $\hat{A}\hat{B}$ is not Hermitian.

2. $\left(\hat{A}\hat{B} + \hat{B}\hat{A}\right)^+ = \hat{B}\hat{A} + \hat{A}\hat{B}$ is Hermitian.

3. If $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$=0, then $\hat{A}\hat{B}$ is Hermitian, since $\left(\hat{A}\hat{B}\right)^+ = \hat{B}^+\hat{A}^+ = \hat{B}\hat{A}$

4. $\left(\hat{A}^2\right)^+ = \left(\hat{A}\hat{A}\right)^+ = \hat{A}^+\hat{A}^+ = \hat{A}\hat{A} = \hat{A}^2$ is Hermitian.

4.4 Discrete orthogonal basis $\{|\varphi_n\rangle\}$

A discrete set of kets $\{|\varphi_n\rangle\}$ is orthonormal if it satisfies the following relation:

$$\langle \varphi_n | \varphi_m \rangle = \delta_{nm} .$$

A basis $\{|\varphi_n\rangle\}$ is said to form a complete orthonormal basis, if any $|\psi\rangle$ can be expanded uniquely as

$$|\psi\rangle = \sum_n c_n |\varphi_n\rangle .$$

We note that

$$\langle \varphi_n | \psi \rangle = \sum_m c_m \langle \varphi_n | \varphi_m \rangle = \sum_m c_m \delta_{nm} = c_n .$$

Then $|\psi\rangle$ can be rewritten as

$$|\psi\rangle = \sum_n c_n |\varphi_n\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle = (\sum_n |\varphi_n\rangle\langle\varphi_n|)|\psi\rangle .$$

This means that

$$\sum_n |\varphi_n\rangle\langle\varphi_n| = 1 .$$ (**closure relation**, **completeness**)

Here we define the projection operator $\hat{P}_n$ as

$$\hat{P}_n = |\varphi_n\rangle\langle\varphi_n| .$$

where

$$\sum_n \hat{P}_n = \sum_n |\varphi_n\rangle\langle\varphi_n| = \hat{1}$$ (closure relation)

This operator is a Hermitian operator, since

$$\hat{P}_n^{\,+} = |\varphi_n\rangle\langle\varphi_n| = \hat{P}_n .$$

We also have the relation,

$$\hat{P}_n^{\,2} = (|\varphi_n\rangle\langle\varphi_n|)(|\varphi_n\rangle\langle\varphi_n|) = \hat{P}_n .$$

4.5 Matrix element of $\hat{A}^+$

For any operator $\hat{A}$ and any basis $\{|\varphi_n\rangle\}$, the matrix element is defined as

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

Since

$$\langle\varphi_n|\hat{A}^+|\varphi_m\rangle = \langle\varphi_m|\hat{A}|\varphi_n\rangle^* ,$$

we have

$$\langle\varphi_n|\hat{A}^+|\varphi_m\rangle = \langle\varphi_m|\hat{A}|\varphi_n\rangle^* .$$

This means that the matrix element of $\hat{A}^+$ is the complex conjugate of the transpose matrix of $\hat{A}$.

The matrix A can be described by

$$\hat{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & . & . & . & . & . & . & . \\ A_{21} & A_{22} & A_{23} & . & . & . & . & . & . & . \\ A_{31} & A_{32} & A_{33} & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \end{pmatrix},$$

and

$$\hat{A}^+ = \left(\hat{A}^T\right)^* = \begin{pmatrix} A_{11}^* & A_{21}^* & A_{31}^* & . & . & . & . & . & . & . \\ A_{12}^* & A_{22}^* & A_{32}^* & . & . & . & . & . & . & . \\ A_{13}^* & A_{23}^* & A_{33}^* & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \end{pmatrix}.$$

Note that the infinite dimensionality of these matrices is a consequence of the infinite dimensionality of Hilbert space. The finite matrices are relevant to vector spaces of finite dimension.

If $\hat{A}$ is Hermitian ($\hat{A}^+ = \hat{A}$), we have

$$A_{nm} = A_{mn}^*.$$

We note that the Hermitian operator is called a observable. For $n = m$ (diagonal element), $A_{nn} = A_{nn}^*$, implying that A_{nn} is always real numbers.

4.6 Representation of ket (column matrix)

In a discrete orthogonal basis $\{|\varphi_n\rangle\}$, a ket $|\psi\rangle$ is represented by the set of numbers c_n;

$$|\psi\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle = \sum_n c_n|\varphi_n\rangle = \begin{pmatrix} c_1 \\ c_2 \\ . \\ . \\ . \end{pmatrix},|$$

where

$$c_n = \langle\varphi_n|\psi\rangle.$$

These numbers can be arranged vertically , forming a column matrix,

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ . \\ . \\ . \\ . \end{pmatrix} = \begin{pmatrix} <\varphi_1|\psi> \\ <\varphi_2|\psi> \\ <\varphi_3|\psi> \\ . \\ . \\ . \\ . \end{pmatrix}.$$

4.7 Representation of bras (row matrix)

A bra $\langle\psi|$ can be represented by the set of numbers $c_n^* = \langle\varphi_n|\psi\rangle^* = \langle\psi|\varphi_n\rangle$

$$\langle\psi| = \sum_n \langle\psi|\varphi_n\rangle\langle\varphi_n| = \sum_n c_n^*\langle\varphi_n|.$$

Let us arrange the components c_n^* of the bra $\langle\psi|$ horizontally, forming a row matrix,

$$\langle\psi| = \begin{pmatrix} c_1^* & c_2^* & c_3^* & . & . & . & . \end{pmatrix} = \begin{pmatrix} \langle\varphi_1|\psi\rangle^* & \langle\varphi_2|\psi\rangle^* & \langle\varphi_3|\psi\rangle^* & . & . & . & . \end{pmatrix}.$$

4.8 Representation of product of operators

Using the closure relation, we calculate the matrix element of the product $\hat{A}\hat{B}$ in the $\{|\varphi_n\rangle\}$ basis.

$$\langle\varphi_n|\hat{A}\hat{B}|\varphi_m\rangle = \sum_k \langle\varphi_n|\hat{A}|\varphi_k\rangle\langle\varphi_k|\hat{B}|\varphi_m\rangle = \sum_k A_{nk}B_{km} .$$

In the matrix representation, we have

$$\hat{A}\hat{B} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & . & . & . & . & . & . & . & . \\ A_{21} & A_{22} & A_{23} & . & . & . & . & . & . & . & . \\ A_{31} & A_{32} & A_{33} & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} & B_{13} & . & . & . & . & . & . & . & . \\ B_{21} & B_{22} & B_{23} & . & . & . & . & . & . & . & . \\ B_{31} & B_{32} & B_{33} & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . \end{pmatrix} .$$

4.9 Matrix representation of $\hat{A}|\psi\rangle$

We consider a relation

$$|\psi'\rangle = \hat{A}|\psi\rangle$$

where A is an arbitrary operator. The kets $|\psi'\rangle$ and $|\psi\rangle$ are expanded in terms of $\{|\varphi_n\rangle$,

$$|\psi'\rangle = \sum_n c_n'|\varphi_n\rangle = \begin{pmatrix} c_1' \\ c_2' \\ . \\ . \\ . \end{pmatrix}$$

and

$$|\psi\rangle = \sum_n c_n|\varphi_n\rangle = \begin{pmatrix} c_1 \\ c_2 \\ . \\ . \\ . \end{pmatrix}$$

with

$$c_n' = \langle \varphi_n | \psi' \rangle = \sum_m \langle \varphi_n | \hat{A} | \varphi_m \rangle \langle \varphi_m | \psi \rangle .$$

Then we have the matrix representation as

$$|\psi'\rangle = \begin{pmatrix} c_1' \\ c_2' \\ . \\ . \\ . \\ . \\ . \end{pmatrix} = \hat{A}|\psi\rangle = \begin{pmatrix} A_{11} & A_{12} & . & . & . & . & . \\ A_{21} & A_{22} & . & . & . & . & . \\ A_{31} & A_{32} & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ . \\ . \\ . \\ . \\ . \end{pmatrix}$$

4.10 Expression for the number $\langle \varphi | \hat{A} | \psi \rangle$

$$\begin{aligned} \langle \varphi | \hat{A} | \psi \rangle &= \sum_{n.m} \langle \varphi | \varphi_n \rangle \langle \varphi_n | \hat{A} | \varphi_m \rangle \langle \varphi_n | \psi \rangle \\ &= \sum_{n.m} b_n^{\ *} A_{nm} c_m \\ &= \begin{pmatrix} b_1^* & b_2^* & b_3^* & . & . & . & . \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & . & . & . & . & . \\ A_{21} & A_{22} & . & . & . & . & . \\ A_{31} & A_{32} & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ . \\ . \\ . \\ . \\ . \end{pmatrix}, \end{aligned}$$

where

$$b_i = \langle \varphi_i | \varphi \rangle, \qquad a_i = \langle \varphi_i | \psi \rangle .$$

4.11 Matrix presentation of outer product

$$|\psi\rangle\langle\varphi| = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ . \\ . \\ . \\ . \end{pmatrix} \begin{pmatrix} b_1^* & b_2^* & b_3^* & . & . & . & . \end{pmatrix} = \begin{pmatrix} c_1b_1^* & c_1b_2^* & c_1b_3^* & . & . & . & . \\ c_2b_1^* & c_2b_2^* & c_2b_3^* & . & . & . & . \\ c_3b_1^* & c_3b_2^* & c_3b_3^* & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{pmatrix}.$$

4.12 Definition of unitary operator

If the Hermitian conjugate ($\hat{U}^+$) of an operator $\hat{U}$ is equal to $\hat{U}^{-1}$, i.e.,

$$\hat{U}^+ = \hat{U}^{-1},$$

then $\hat{U}$ is said to be unitary. This equation can be rewritten as

$$\hat{U}\hat{U}^+ = \hat{U}^+\hat{U} = \hat{1}.$$

4.13 Matrix representation of unitary operator $\hat{U}$

We consider the transformation of the state vectors

$$|\psi'\rangle = \hat{U}|\psi\rangle, \qquad |\varphi'\rangle = \hat{U}|\varphi\rangle,$$

with the unitary operator $\hat{U}$. The unitary transformation preserves the length of vectors and the angle between vectors.

$$\langle\varphi'|\psi'\rangle = \langle\varphi|\hat{U}^+\hat{U}|\psi\rangle = \langle\varphi|\psi\rangle.$$

In the orthogonal basis $\{|\varphi_n\rangle\}$, we have

$$\langle\varphi_n|\hat{U}^+\hat{U}|\varphi_m\rangle = \langle\varphi_n|\varphi_m\rangle.$$

The matrix representation of this expression is given by

$$
\begin{pmatrix}
U_{11}^* & U_{21}^* & . & . & . & U_{n1}^* & . \\
U_{12}^* & U_{22}^* & . & . & . & U_{n2}^* & . \\
. & . & . & . & . & . & . \\
. & . & . & . & . & . & .. \\
. & . & . & . & . & . & . \\
U_{1n}^* & U_{2n}^* & . & . & . & U_{nn}^* & . \\
. & . & . & . & . & . & .
\end{pmatrix}
\begin{pmatrix}
U_{11} & U_{12} & . & . & . & U_{1n} & . \\
U_{21} & U_{22} & . & . & . & U_{2n} & . \\
. & . & . & . & . & . & . \\
. & . & . & . & . & . & .. \\
. & . & . & . & . & . & . \\
U_{n1} & U_{n2} & . & . & . & U_{nn} & . \\
. & . & . & . & . & . & .
\end{pmatrix}
=
\begin{pmatrix}
1 & 0 & . & . & . & 0 & . \\
0 & 1 & . & . & . & 0 & . \\
. & . & . & . & . & . & . \\
. & . & . & . & . & . & .. \\
. & . & . & . & . & . & . \\
0 & 0 & . & . & . & 1 & . \\
. & . & . & . & . & . & .
\end{pmatrix},
$$

where

$$
\hat{U} =
\begin{pmatrix}
U_{11} & U_{12} & . & . & . & U_{1n} & . \\
U_{21} & U_{22} & . & . & . & U_{2n} & . \\
. & . & . & . & . & . & . \\
. & . & . & . & . & . & .. \\
. & . & . & . & . & . & . \\
U_{n1} & U_{n2} & . & . & . & U_{nn} & . \\
. & . & . & . & . & . & .
\end{pmatrix},
$$

and

$$
\hat{U}^+ =
\begin{pmatrix}
U_{11}^* & U_{21}^* & . & . & . & U_{n1}^* & . \\
U_{12}^* & U_{22}^* & . & . & . & U_{n2}^* & . \\
. & . & . & . & . & . & . \\
. & . & . & . & . & . & .. \\
. & . & . & . & . & . & . \\
U_{1n}^* & U_{2n}^* & . & . & . & U_{nn}^* & . \\
. & . & . & . & . & . & .
\end{pmatrix}.
$$

4.14 Unitary-similarity transformation

We consider the relation

$$
|\psi_b\rangle = \hat{A}|\psi_a\rangle, \qquad |\psi_b'\rangle = \hat{A}|\psi_a'\rangle,
$$

where

$$
|\psi_a'\rangle = \hat{U}|\psi_a\rangle,
$$

$$
|\psi_b'\rangle = \hat{U}|\psi_b\rangle,
$$

Then we have

$$|\psi_b'\rangle \equiv \hat{A}'|\psi_a'\rangle = \hat{U}|\psi_b\rangle = \hat{U}\hat{A}|\psi_a\rangle = \hat{U}\hat{A}\hat{U}^{-1}|\psi_a'\rangle,$$

or

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

This equation describes how an operator transforms under a change of basis, is called a unitary-similarity transformation.

4.15 Eigenvalue and eigenvector

We consider the eigenvalue problem given by

$$\hat{A}|a_n\rangle = a_n|a_n\rangle,$$

where

$$\hat{A}^{+} = \hat{A}. \qquad \text{(Hermitian operator)}$$

$|a_n\rangle$ is the eigenket belonging to the eigenvalue a_n. Then we have

$$\langle a_m|\hat{A}|a_n\rangle^{*} = \langle a_n|\hat{A}^{+}|a_m\rangle = \langle a_n|\hat{A}|a_m\rangle,$$

or

$$\langle a_m|a_n|a_n\rangle^{*} = a_n^{*}\langle a_n|a_m\rangle = a_m\langle a_n|a_m\rangle. \qquad (1)$$

(1) *The eigen value is real.*

For $m = n$ in Eq.(1), we have

$$(a_n^{*} - a_n)\langle a_n|a_n\rangle = 0.$$

Since $\langle a_n|a_n\rangle \neq 0$, we get

$$a_n^{*} = a_n.$$

Thus a_n is real.

(2) *The eigenkets are orthogonal.*

In Eq.(1), we have

$$(a_n - a_m)\langle a_n | a_m \rangle = 0 .$$

If $a_n \neq a_m$ (non-degenerate case),

$$\langle a_n | a_m \rangle = 0 \text{ (orthogonal).}$$

For convenience we assume that

$$\langle a_n | a_m \rangle = \delta_{n,m} . \qquad \text{(Kronecker delta)}$$

(3) *The eigenkets of $\hat{A}$ form a complete set.*
For any $|\psi\rangle$, $|\psi\rangle$ can be expressed by

$$|\psi\rangle = \sum_{n=1}^{\infty} c_n |a_n\rangle ,$$

with

$$c_n = \langle a_n | \psi \rangle .$$

((Closure relation))

$$|\psi\rangle = \sum_{n=1}^{\infty} c_n |a_n\rangle = \sum_{n=1}^{\infty} |a_n\rangle\langle a_n | \psi\rangle .$$

Because $|\psi\rangle$ is an arbitrary ket, we must have

$$\sum_{n=1}^{\infty} |a_n\rangle\langle a_n| = \hat{1} .$$

For $\hat{A}$ with $\hat{A}|a_n\rangle = a_n |a_n\rangle$, we have

$$\hat{A} = \hat{A}\sum_{n=1}^{\infty} |a_n\rangle\langle a_n| = \sum_{n=1}^{\infty} \hat{A}|a_n\rangle\langle a_n| = \sum_{n=1}^{\infty} a_n |a_n\rangle\langle a_n| .$$

4.16 Measurement

$|\psi\rangle$ is the state and $\hat{A}$ is an operator.

Before a measurement of observable (Hermitian operator) $\hat{A}$ is made, the system is assumed to be represented by some linear combination.

$$|\psi\rangle = \sum_n c_n |a_n\rangle,$$

where

$$c_n = \langle a_n|\psi\rangle.$$

When the measurement is performed, the system is thrown into one of the eigenststes, $|a_n\rangle$;

$$\hat{A}|a_n\rangle = a_n|a_n\rangle \qquad \text{(eigenvalue problem)}$$

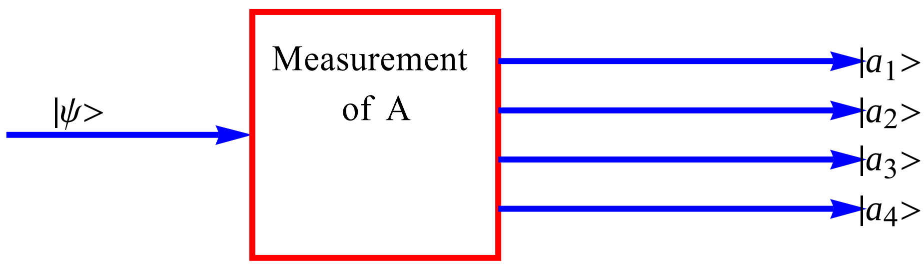


Fig. Measurement of observable A.

The state $|\psi\rangle$ can be expressed in terms of the eigenket $\{|a_n\rangle\}$ as

$$|\psi\rangle = (\sum_{n=1}^{\infty}|a_n\rangle\langle a_n|)|\psi\rangle = \sum_{n=1}^{\infty}|a_n\rangle\langle a_n|\psi\rangle \qquad \text{(closure relation)}$$

The probability of finding $|a_n\rangle$ is given by

$$P(a_n) = |\langle a_n|\psi\rangle|^2$$

4.17 Change of basis

We want to know the eigenket of $|a_n\rangle$ with the eigenvalue a_n:

$$\hat{A}|a_n\rangle = a_n|a_n\rangle. \qquad \text{(eigenvalue problem)}$$

Suppose that A_{nm} is the matrix element of $\hat{A}$ on the basis $\{|b_n\rangle\}$

$$A_{nm} = \langle b_n | \hat{A} | b_m \rangle$$

$$\hat{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & . & . & . \\ A_{21} & A_{22} & A_{23} & . & . & . \\ A_{31} & A_{32} & A_{33}. & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{pmatrix}$$

under the basis $\{|b_n\rangle\}$,

$$|b_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ . \\ . \\ 0 \end{pmatrix}, \qquad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ . \\ . \\ 0 \end{pmatrix}, \ldots\ldots$$

Note that $|a_n\rangle$ is related to $|b_n\rangle$ through the unitary operator $\hat{U}$ by

$$|a_n\rangle = \hat{U}|b_n\rangle, \qquad |b_n\rangle = \hat{U}^{-1} = \hat{U}^{+}|b_n\rangle$$

or

$$\langle a_n | = \langle b_n | \hat{U}^{+}$$

The unitary operator satisfies the condition,

$$\hat{U}^{+}\hat{U} = \hat{1}.$$

Note that

$$\langle a_n | a_m \rangle = \langle b_n | \hat{U}^{+}\hat{U} | b_m \rangle = \langle b_n | \hat{1} | b_m \rangle = \langle b_n | b_m \rangle = \delta_{n,m}$$

with

$$\hat{U} = \hat{U}\sum_n |b_n\rangle\langle b_n|$$
$$= \sum_n \hat{U}|b_n\rangle\langle b_n| = \sum_n |a_n\rangle\langle b_n| \qquad \text{(closure relation).}$$

and

$$\hat{U}^+ = \sum_n \hat{U}^+|a_n\rangle\langle a_n| = \sum_n |b_n\rangle\langle a_n|,$$

where δ_{nm} is the Kronecker-delta, and $\delta_{\text{nm}} = 1$ for $n = m$, 0 otherwise.

Using the expressions of $\hat{U}$ and $\hat{U}^+$, we have

(1):

$$\hat{U}^+\hat{U} = \sum_m |b_m\rangle\langle a_m|\sum_n |a_n\rangle\langle b_n| = \sum_{m,n} |b_m\rangle\langle a_m|a_n\rangle\langle b_n| = \sum_{m,n} |b_m\rangle\delta_{mn}\langle b_n| = \hat{1}$$

$$\hat{U}\hat{U}^+ = \sum_m |a_m\rangle\langle b_m|\sum_n |b_n\rangle\langle a_n| = \sum_{m,n} |a_m\rangle\langle b_m|b_n\rangle\langle a_n| = \sum_{m,n} |a_m\rangle\delta_{mn}\langle a_n| = \hat{1}$$

(2):

$$\hat{A}|a_n\rangle = a_n|a_n\rangle, \qquad |a_n\rangle = \hat{U}|b_n\rangle$$

Then we have

$$\hat{U}^+\hat{A}\hat{U}|b_n\rangle = a_n|b_n\rangle$$

In other words, $\hat{U}^+\hat{A}\hat{U}$ should be a diagonal matrix;

$$\hat{U}^+\hat{A}\hat{U} = \sum_n |b_n\rangle\langle a_n|\hat{A}\sum_m |a_m\rangle\langle b_n| = \sum_n a_n|b_n\rangle\langle b_n|$$

or

$$\hat{U}^+\hat{A}\hat{U}|b_k\rangle = \sum_n |b_n\rangle\langle a_n|\hat{A}\sum_m |a_m\rangle\langle b_n|b_k\rangle = \sum_n a_n|b_n\rangle\langle b_n|b_k\rangle = a_k|b_k\rangle$$

or

$$\hat{U}^+\hat{A}\hat{U} = \begin{pmatrix} a_1 & 0 & 0 & . & . & 0 \\ 0 & a_2 & 0 & . & . & 0 \\ 0 & 0 & a_3 & . & . & 0 \\ . & . & . & . & . & 0 \\ . & . & . & . & . & 0 \\ 0 & . & . & . & . & a_{nn} \end{pmatrix}$$

where the basis is $\{|b_n\rangle\}$.

4.18 Eigenvalue problem: formulation

This problem is reduced to the determination of the matrix element of $\hat{U}$ in the basis of $\{|b_n\rangle\}$.

$$\hat{A}|a_m\rangle = a_m|a_m\rangle$$

with $|a_m\rangle = \hat{U}|b_m\rangle$. We note that

$$\langle b_n|\hat{A}|a_m\rangle = a_m\langle b_n|a_m\rangle,$$

or

$$\langle b_n|\hat{A}\hat{U}|b_m\rangle = a_m\langle b_n|\hat{U}|b_m\rangle .$$

Then we have the matrix representation,

$$\sum_k \langle b_n|\hat{A}|b_k\rangle\langle b_k|\hat{U}|b_m\rangle = a_m\langle b_n|\hat{U}|b_m\rangle ,$$

or

$$\sum_k A_{nk}U_{km} = a_m U_{nm}$$

For the eigenvalue $\lambda = a_m$

$$\begin{pmatrix} A_{11} & A_{12} & . & . & . & A_{1n} & . \\ A_{21} & A_{22} & . & . & . & A_{2n} & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ A_{n1} & A_{n2} & . & . & . & A_{nn} & . \\ . & . & . & . & . & . & . \end{pmatrix}\begin{pmatrix} U_{1m} \\ U_{2m} \\ . \\ . \\ . \\ U_{nm} \\ . \end{pmatrix} = a_m \begin{pmatrix} U_{1m} \\ U_{2m} \\ . \\ . \\ . \\ U_{nm} \\ . \end{pmatrix}$$

and

$$\left|a_m\right\rangle = \hat{U}\left|b_m\right\rangle = \begin{pmatrix} U_{11} & U_{12} & . & . & . & U_{1n} & . \\ U_{21} & U_{22} & . & . & . & U_{2n} & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & .. \\ . & . & . & . & . & . & . \\ U_{n1} & U_{n2} & . & . & . & U_{nn} & . \\ . & . & . & . & . & . & . \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ . \\ . \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{1m} \\ U_{2m} \\ . \\ . \\ . \\ U_{nm} \\ . \end{pmatrix}$$

where

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} & . & . & . & U_{1n} & . \\ U_{21} & U_{22} & . & . & . & U_{2n} & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & .. \\ . & . & . & . & . & . & . \\ U_{n1} & U_{n2} & . & . & . & U_{nn} & . \\ . & . & . & . & . & . & . \end{pmatrix}$$

$$\left|a_m\right\rangle = \hat{U}\left|b_m\right\rangle = U_{1m}\left|b_1\right\rangle + U_{2m}\left|b_2\right\rangle + ... + U_{nm}\left|b_n\right\rangle + ...$$

Note that $\hat{U}^{+}\hat{A}\hat{U}$ is a diagonal matrix given by

$$\hat{U}^{+}\hat{A}\hat{U} = \begin{pmatrix} a_1 & 0 & . & . & . & 0 & . \\ 0 & a_2 & . & . & . & 0 & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & . & . & . & a_n & . \\ . & . & . & . & . & . & . \end{pmatrix} \qquad \text{(diagonal matrix).}$$

under the basis of $\{|b_n\rangle\}$.

4.19 Expression of operators, ket, bra and so on (Mathematica; Method-I)

The method-I described here is the same as that in the standard textbook of mathemtica. However, it is sometimes inconvenient for one to make a Mathemtica program to solve problems.

You need to put the definition of complex conjugate "*" in your program .

SuperStar; expr_* := expr /. Complex[a_, b_] :→ Complex[a, -b)]

For matrix $\hat{A}$ (for example 3x3), type as

$\hat{A} = \{\{A_{11}, A_{12}, A_{13}\}, \{A_{21}, A_{22}, A_{23}\}, \{A_{31}, A_{32}, A_{33}\}\}$.

$\hat{A}$//MatrixForm:

$$\hat{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}.$$

For $\hat{A}^{+}$ (Hermite conjugate of $\hat{A}$), type as

$\hat{A}^{+}$= Transpose[$\hat{A}^{*}$],

$\hat{A}^{+}$//MatrixForm,

$$\hat{A}^{+} = \begin{pmatrix} A_{11}^{*} & A_{21}^{*} & A_{31}^{*} \\ A_{12}^{*} & A_{22}^{*} & A_{23}^{*} \\ A_{13}^{*} & A_{23}^{*} & A_{33}^{*} \end{pmatrix}.$$

For the ket vector $|\psi\rangle$ (for the column matrix), type as

$|\psi\rangle = \{\{a_1\},\{a_2\},\{a_3\}\}$,

$|\psi\rangle$//MatrixForm,

$$|\psi\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}.$$

For the bra vector $\langle\psi|$ (for the row matrix), type as

$\langle\psi|$=Transpose[a*]={{$a_1{}^*$,$a_2{}^*$,$a_3{}^*$}},

which is the Hermitian conjugate of $|\psi\rangle$.

$\langle\psi|$//MatrixForm,

$$\langle\psi| = \begin{pmatrix} a_1{}^* & a_2{}^* & a_3{}^* \end{pmatrix}.$$

For the calculation of $\hat{A}|\psi\rangle$, type $\hat{A}.|\psi\rangle$

$\hat{A}\cdot|\psi\rangle$//MatrixForm,

$$\hat{A}|\psi\rangle = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}.$$

Note that "." in $\hat{A}.|\psi\rangle$ is a period "."

For the calculation of $\langle\psi|\hat{A}$, type $(\langle\psi|).\hat{A}$

$\langle\psi|\hat{A}$//MatrixForm,

$$\langle\psi|\hat{A} = \begin{pmatrix} a_1{}^* & a_2{}^* & a_3{}^* \end{pmatrix}\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}.$$

For the calculation of $\langle\psi|A|\varphi\rangle$, type as $\langle\psi|\hat{A}|\varphi\rangle$

$$\langle\psi|\hat{A}|\varphi\rangle = \begin{pmatrix} a_1^* & a_2^* & a_3^* \end{pmatrix}\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix},$$

where

$$|\varphi\rangle = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}.$$

For the operator $|\psi\rangle\langle\varphi|$, type $|\psi\rangle.\langle\varphi|$

$|\psi\rangle\langle\varphi|$ //MatrixForm,

$$|\psi\rangle\langle\varphi| = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}\begin{pmatrix} b_1^* & b_2^* & b_3^* \end{pmatrix} = \begin{pmatrix} a_1 b_1^* & a_1 b_2^* & a_1 b_3^* \\ a_2 b_1^* & a_2 b_2^* & a_2 b_3^* \\ a_3 b_1^* & a3 b_2^* & a_3 b_3^* \end{pmatrix}.$$

((**Mathematica**))

```
Clear["Global`*"]
```

A matrix A:

```
A = {{A11, A12, A13}, {A21, A22, A23},
   {A31, A32, A33}};
```

```
A // MatrixForm
```

$$\begin{pmatrix} A11 & A12 & A13 \\ A21 & A22 & A23 \\ A31 & A32 & A33 \end{pmatrix}$$

A column matrix ψ

```
ψ = {{a1}, {a2}, {a3}};
```

```
ψ // MatrixForm
```

$$\begin{pmatrix} a1 \\ a2 \\ a3 \end{pmatrix}$$

Calculation of A | ψ >

```
A.ψ
```

```
{{a1 A11 + A12 a2 + A13 a3},
 {a1 A21 + a2 A22 + A23 a3}, {a1 A31 + a2 A32 + a3 A33}}
```

```
Clear["Global`*"]
```

A matrix A:

```
A = {{A11, A12, A13}, {A21, A22, A23},
   {A31, A32, A33}};
```

A column matrix ψ

```
ψ = {a1, a2, a3};
```

Calculation of A | ψ >

```
A.ψ
```

```
{a1 A11 + A12 a2 + A13 a3,
 a1 A21 + a2 A22 + A23 a3, a1 A31 + a2 A32 + a3 A33}
```

A row matrix ϕ,
b1cc means the complex conjugate of b1, and so on

```
ϕcc = {b1cc, b2cc, b3cc};
```

Inner product <ϕ|ψ>

```
ϕcc.ψ
```

```
a1 b1cc + a2 b2cc + a3 b3cc
```

Outer product |ψ><ϕ|

```
Outer[Times, ψ, ϕcc]
```

```
{{a1 b1cc, a1 b2cc, a1 b3cc},
 {a2 b1cc, a2 b2cc, a2 b3cc},
 {a3 b1cc, a3 b2cc, a3 b3cc}}
```

Matrix element <ϕ|A|ψ>

```
ϕ.A.ψ // Expand
```

```
ϕ.{a1 A11 + A12 a2 + A13 a3,
   a1 A21 + a2 A22 + A23 a3, a1 A31 + a2 A32 + a3 A33}
```

4.20 Mathematica Method II

The method I described above is very precise mathematically, but it is not so convenient. Hereafter we use simpler method (Method-II) which is described in the following way.

For the ket vector $|\psi\rangle$, simply type as

$$|\psi\rangle = \psi = \{a_1, a_2, a_3\}.$$

For the bra vector $\langle\varphi|$, simply type as

$$\langle\varphi| = \varphi^* = \{b_1^*, b_2^*, b_3^*\}.$$

The inner product $\langle\varphi|\psi\rangle$ is given by $\varphi^*.\psi$. How about the outer product ($|\psi\rangle\langle\phi|$)? We can use the program

Outer[Times, ψ, φ^*]

4.21 Mathematica (method II)

```
Clear["Global`*"]
```

A matrix A:

```
A = {{A11, A12, A13}, {A21, A22, A23},
   {A31, A32, A33}};
```

A column matrix ψ

```
ψ = {a1, a2, a3};
```

Calculation of A | ψ >

```
A.ψ
```

```
{a1 A11 + A12 a2 + A13 a3,
 a1 A21 + a2 A22 + A23 a3, a1 A31 + a2 A32 + a3 A33}
```

A row matrix ϕ,
b1cc means the complex conjugate of b1.
b2cc means the complex conjugate of b2.

```
ϕ = {b1cc, b2cc, b3cc};
```

Inner product <ϕ|ψ>

```
ϕ.ψ
```

```
a1 b1cc + a2 b2cc + a3 b3cc
```

Matrix element <ϕ|A|ψ>

```
ϕ.A.ψ // Expand
```

```
a1 A11 b1cc + A12 a2 b1cc + A13 a3 b1cc +
 a1 A21 b2cc + a2 A22 b2cc + A23 a3 b2cc +
 a1 A31 b3cc + a2 A32 b3cc + a3 A33 b3cc
```

4.22 Griffiths; Problem 3-9, p.86 Method-II

Given the following two matrices

$$\hat{A} = \begin{pmatrix} -1 & 1 & i \\ 2 & 0 & 3 \\ 2i & -2i & 2 \end{pmatrix}, \qquad \hat{B} = \begin{pmatrix} 2 & 0 & -i \\ 0 & 1 & 0 \\ i & 3 & 2 \end{pmatrix}$$

Compute

(i) $\hat{A} + \hat{B}$
(ii) $\hat{A}\hat{B}$
(iii) $[\hat{A}, \hat{B}]$
(iv) $\tilde{A}$ (transpose of $\hat{A}$)
(v) $\hat{A}^*$
(vi) $\hat{A}^+$
(vii) $Tr(\hat{B})$
(viii) $\det(\hat{B})$
(ix) $\hat{B}^{-1}$. Check that $\hat{B}\hat{B}^{-1} = \hat{1}$. Does $\hat{A}$ have an inverse?

((**Mathematica**))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
```

$$A = \begin{pmatrix} -1 & 1 & i \\ 2 & 0 & 3 \\ 2i & -2i & 2 \end{pmatrix};$$

$$B = \begin{pmatrix} 2 & 0 & -i \\ 0 & 1 & 0 \\ i & 3 & 2 \end{pmatrix};$$

```
A + B // MatrixForm
```

$$\begin{pmatrix} 1 & 1 & 0 \\ 2 & 1 & 3 \\ 3i & 3-2i & 4 \end{pmatrix}$$

```
A.B // MatrixForm
```

$$\begin{pmatrix} -3 & 1+3i & 3i \\ 4+3i & 9 & 6-2i \\ 6i & 6-2i & 6 \end{pmatrix}$$

```
A.B - B.A // MatrixForm
```

$$\begin{pmatrix} -3 & 1+3i & 3i \\ 2+3i & 9 & 3-2i \\ -6+3i & 6+i & -6 \end{pmatrix}$$

```
Transpose[A] // MatrixForm
```

$$\begin{pmatrix} -1 & 2 & 2i \\ 1 & 0 & -2i \\ i & 3 & 2 \end{pmatrix}$$

```
A* // MatrixForm
```

$$\begin{pmatrix} -1 & 1 & -i \\ 2 & 0 & 3 \\ -2i & 2i & 2 \end{pmatrix}$$

```
AH = ConjugateTranspose[A] // MatrixForm
```

$$\begin{pmatrix} -1 & 2 & -2i \\ 1 & 0 & 2i \\ -i & 3 & 2 \end{pmatrix}$$

```
{Tr[A], Tr[B]}
```

```
{1, 5}
```

```
{Det[A], Det[B]}
```

```
{0, 3}
```

```
Inverse[B] // MatrixForm
```

$$\begin{pmatrix} \frac{2}{3} & -i & \frac{i}{3} \\ 0 & 1 & 0 \\ -\frac{i}{3} & -2 & \frac{2}{3} \end{pmatrix}$$

```
Inverse[A]
```

Inverse::sing : Matrix {{−1, 1, i}, {2, 0, 3}, {2 i, −2 i, 2}} is singular. ≫

```
Inverse[{{-1, 1, i}, {2, 0, 3}, {2 i, -2 i, 2}}]
```

4.23 Griffiths;Problem 3-10, p.86 Method II

$$|a\rangle = \begin{pmatrix} i \\ 2i \\ 2 \end{pmatrix}, \qquad |b\rangle = \begin{pmatrix} 2 \\ 1-i \\ 0 \end{pmatrix}, \qquad \hat{A} = \begin{pmatrix} -1 & 1 & i \\ 2 & 0 & 3 \\ 2i & -2i & 2 \end{pmatrix}, \qquad \hat{B} = \begin{pmatrix} 2 & 0 & -i \\ 0 & 1 & 0 \\ i & 3 & 2 \end{pmatrix}$$

Find

(i) $\hat{A}|a\rangle$
(ii) $\langle a|b\rangle$
(iii) $\langle a|\hat{B}|b\rangle$
(iv) $|a\rangle\langle b|$

((**Mathematica**))

```
Clear["Global`*"]

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
```

$$a = \{i, 2i, 2\};\ b = \{2, 1-i, 0\};\ A = \begin{pmatrix} -1 & 1 & i \\ 2 & 0 & 3 \\ 2i & -2i & 2 \end{pmatrix};$$

$$B = \begin{pmatrix} 2 & 0 & -i \\ 0 & 1 & 0 \\ i & 3 & 2 \end{pmatrix};$$

```
A.a // MatrixForm
```

$$\begin{pmatrix} 3i \\ 6+2i \\ 6 \end{pmatrix}$$

```
a*
```

{-i, -2 i, 2}

```
a*.b
```

-2 - 4 i

```
a*.B.b
```

4 - 8 i

```
Outer[Times, a, b*]
```

{{2 i, -1 + i, 0}, {4 i, -2 + 2 i, 0}, {4, 2 + 2 i, 0}}

4.24 Solving the eigenvalue problem (Mathematica, method-II):

4.24.1 General case

Here we discuss the case of nondegenerate system, where the eigenvalues are discrete different values.

(1) Get the matrix of $\hat{A}$ with the element of $\langle b_n|\hat{A}|b_m\rangle$.

A={{A_{11}, A_{12}, A_{13},....},{A_{21}, A_{22}, A_{23},....},{A_{31}, A_{32}, A_{33},....},...}}

(2) Use Mathematica to calculate the eigenvalues and the normalized eigenkets.

Using the Mathematica program

Eigensystem[A]

one can get the eigenvalues and eigenvectors.

{a_1, a_2, a_3,…., a_m,…, $|\varphi_1\rangle$, $|\varphi_2\rangle$, $|\varphi_3\rangle$,…..}

Using the Mathematica program

Normalize[$|\varphi_m\rangle$]

one can get the normalized eigenket,

$$|\varphi_m\rangle = \begin{pmatrix} U_{1m} \\ U_{2m} \\ . \\ . \\ . \\ U_{nm} \\ . \end{pmatrix}$$

for $\lambda = a_m$, where $\langle\varphi_m|\varphi_m\rangle = 1$. Determine the values of U_{nm} (n = 1, 2, 3, …..) for $\lambda = a_m$. Make sure that

$$\langle\varphi_n|\varphi_m\rangle = \delta_{nm}.$$

(3) Determine the unitary matrices $\hat{U}$ and $\hat{U}^+$.

$$\hat{U}^T = \{|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, ...\}$$
$$= \begin{pmatrix} U_{11} & U_{21} & U_{31} & . & . & . \\ U_{12} & U_{22} & U_{32} & . & . & . \\ U_{13} & U_{23} & U_{33} & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{pmatrix}$$

$$\hat{U} = Transpose[U^T] = \begin{pmatrix} U_{11} & U_{12} & U_{13} & . & . & . \\ U_{21} & U_{22} & U_{23} & . & . & . \\ U_{31} & U_{32} & U_{33} & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{pmatrix}$$

and

$$\hat{U}^+ = (U^T)^* = \begin{pmatrix} U_{11}^* & U_{21}^* & U_{31}^* & . & . & . \\ U_{12}^* & U_{22}^* & U_{32}^* & . & . & . \\ U_{13}^* & U_{23}^* & U_{33}^* & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{pmatrix}$$

(4) One may need to make sure that $\hat{U}^+\hat{A}\hat{U}$ is a diagonal matrix;

$$\hat{U}^+\hat{A}\hat{U} = \begin{pmatrix} a_1 & 0 & 0 & . & . & . \\ 0 & a_2 & 0 & . & . & . \\ 0 & 0 & a_3 & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{pmatrix}$$

4.24-2 3x3 matrices

The eigenvalue problem can be solved as follows using the method-II. For simplicity, we assume that $\hat{A}$ is a 3x3 matrix (Hermitian).

The matrix A is typed as

$\hat{A}$={{A$_{11}$, A$_{12}$, A$_{13}$}, {A$_{21}$, A$_{22}$, A$_{23}$},{A$_{31}$, A$_{32}$, A$_{33}$}}

Type Eigensystem[$\hat{A}$].

You will find the following message in the computer.

$\{\{a_1, a_2, a_3\}, \{|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle\}\}$

where $|\psi_i\rangle$ is the eigenvector of $\hat{A}$ with eigenvalue a_i (i = 1, 2, 3). For the nondegenerate case, the eigenvalues are different real values.

$|\varphi_i\rangle$ is the normalized eigenket and can be calculated as

$|\varphi_1\rangle = Normalize[|\psi_1\rangle] = \{U_{11}, U_{21}, U_{31}\}$ or φ_1

$|\varphi_2\rangle = Normalize[|\psi_2\rangle] = \{U_{12}, U_{22}, U_{32}\}$ or φ_2

$|\varphi_3\rangle = Normalize[|\psi_3\rangle] = \{U_{13}, U_{23}, U_{33}\}$ or φ_3

U_{ij} is the matrix element of the unitary operator (matrix). We need to make sure that $\{\varphi_1^*.\varphi_2, \varphi_2^*.\varphi_3, \varphi_3^*.\varphi_1\}$ is equal to {0, 0, 0,}. The unitary operator (matrix) is obtained as follows.

$\hat{U}^T = \{|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle\}$.

$\hat{U}^T$ //MatrixForm

$$\hat{U}^T = \begin{pmatrix} U_{11} & U_{21} & U_{31} \\ U_{12} & U_{22} & U_{32} \\ U_{13} & U_{23} & U_{33} \end{pmatrix},$$

or

$\hat{U}$=Transpose[$\hat{U}^T$],

$\hat{U}$ //MatrixForm

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}.$$

$\hat{U}$ is the unitary operator. $\hat{U}^{+}$ (Hermite conjugate) is obtained as

$\hat{U}^{+}$=Transpose[$\hat{U}^{*}$]

$$\hat{U}^{+} = \begin{pmatrix} U_{11}{}^{*} & U_{21}{}^{*} & U_{31}{}^{*} \\ U_{12}{}^{*} & U_{22}{}^{*} & U_{32}{}^{*} \\ U_{13}{}^{*} & U_{23}{}^{*} & U_{33}{}^{*} \end{pmatrix}$$

$\hat{U}^{+}.\hat{A}.\hat{U}$ is a diagonal matrix given by

$$\hat{U}^{+}.\hat{A}.\hat{U} = \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix}$$

and of course, we have

$$\hat{U}^{+}.\hat{U} = \hat{U}.\hat{U}^{+} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

In conclusion, using this method one can calculate any kind of eigenvalue problems (the nondegenerate case).

4.25 Griffiths; Example, p.88 Nondegenerate case

Find the eigenvalues and eigenvectors of the following matrix.

$$\hat{A} = \begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}, \qquad |b_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |b_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

((**Mathematica**))

The matrix $\hat{A}$ is not a Hermitian matrix.

```
Clear["Global`*"];

exp_ * :=
  exp /.
   {Complex[re_, im_] :> Complex[re, -im]};
```

$$A = \begin{pmatrix} 2 & 0 & -2 \\ -2\,i & i & 2\,i \\ 1 & 0 & -1 \end{pmatrix};$$

```
eq1 = Eigensystem[A]
```

{{i, 1, 0},
 {{0, 1, 0}, {2, 1 - i, 1}, {1, 0, 1}}}

```
ψ1 = Normalize[eq1[[2, 1]]]
```

{0, 1, 0}

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$$\left\{\frac{2}{\sqrt{7}}, \frac{1-i}{\sqrt{7}}, \frac{1}{\sqrt{7}}\right\}$$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$$\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$$

```
{A.ψ1 - i ψ1, A.ψ2 - ψ2, A.ψ3}
```

{{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}

Note that ψ1, ψ2, ψ3 do not form an orthnormal set.

```
{ψ1*. ψ2, ψ2*. ψ3, ψ3*. ψ1} // Simplify
```

$$\left\{\frac{1-i}{\sqrt{7}}, \frac{3}{\sqrt{14}}, 0\right\}$$

4.26 Griffiths: Problem 3-22, p.94 Nondegenerate case

$$\hat{A} = \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix}$$

(i) Verify that $\hat{A}$ is Hermitian.
(ii) Find the eigenmvalues (note that they are real).
(iii) Find and normalize the eigenvalues (note that they are orthogonal).
(iv) Construct the Unitary diagonalizing matrix $\hat{U}$ and check explicitly that it diagonalizes $\hat{A}$.
(v) Check that det($\hat{A}$) and Tr($\hat{A}$) are the same for $\hat{A}$ as they are for its diagonalized.

((**Mathematica**))

```
Clear["Global`*"]

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

A = {{1, 1 - i}, {1 + i, 0}};

A // MatrixForm
```

$$\begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix}$$

Is A a Hermitian matrix?

```
HermitianMatrixQ[A]

True

eq1 = Eigensystem[A]

{{2, -1}, {{1 - i, 1}, {-1 + i, 2}}}

a1 = Normalize[eq1[[2, 1]]]
```

$$\left\{\frac{1-i}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}$$

```
a2 = Normalize[eq1[[2, 2]]] // Simplify
```

$$\left\{-\frac{1-i}{\sqrt{6}}, \sqrt{\frac{2}{3}}\right\}$$

Orthogonality

```
a1*.a2 // Simplify

0

UT = {a1, a2}
```

$$\left\{\left\{\frac{1-i}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{-\frac{1-i}{\sqrt{6}}, \sqrt{\frac{2}{3}}\right\}\right\}$$

```
UT // MatrixForm
```

$$\begin{pmatrix} \frac{1-i}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1-i}{\sqrt{6}} & \sqrt{\frac{2}{3}} \end{pmatrix}$$

U is the Unitary operator and UT is the transpose of the Unitary operator

```
U = Transpose[UT]
```

$$\left\{\left\{\frac{1-i}{\sqrt{3}},\ -\frac{1-i}{\sqrt{6}}\right\},\ \left\{\frac{1}{\sqrt{3}},\ \sqrt{\frac{2}{3}}\right\}\right\}$$

```
U // MatrixForm
```

$$\begin{pmatrix} \frac{1-i}{\sqrt{3}} & -\frac{1-i}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \sqrt{\frac{2}{3}} \end{pmatrix}$$

UH is the Hermite conjugate of U

```
UH = Transpose[U*]
```

$$\left\{\left\{\frac{1+i}{\sqrt{3}},\ \frac{1}{\sqrt{3}}\right\},\ \left\{-\frac{1+i}{\sqrt{6}},\ \sqrt{\frac{2}{3}}\right\}\right\}$$

```
UH.A.U // Simplify
```

{{2, 0}, {0, -1}}

```
% // MatrixForm
```

$$\begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}$$

```
Det[A]
```

-2

```
Tr[A]
```

1

4.27 Schaum; Problem 4-17, p.65 Nondegenerate case

Consider a two dimensional physical system. The kets $|b_1\rangle$ and $|b_2\rangle$ form an orthonormal basis of the state space. we define a new basis $|a_1\rangle$ and $|a_2\rangle$ by

$$|a_1\rangle = \frac{1}{\sqrt{2}}(|b_1\rangle + |b_2\rangle), \ |a_2\rangle = \frac{1}{\sqrt{2}}(|b_1\rangle - |b_2\rangle).$$

An operator $\hat{P}$ is represented in the $|b_i\rangle$-basis by the matrix

$$\hat{P} = \begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix}.$$

Find the representation of $\hat{P}$ in the basis $|a_i\rangle$, i.e., find the matrix $\langle a_i|\hat{P}|a_j\rangle$.

((**Solution**))

$$|a_1\rangle = \hat{U}|b_1\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix},$$

$$|a_2\rangle = \hat{U}|b_2\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix},$$

where $\hat{U}$ is the unitary operator.

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$$

$$\hat{U}^+ = \begin{pmatrix} U_{11}{}^* & U_{12}{}^* \\ U_{12}{}^* & U_{22}{}^* \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$$

$$\hat{P} = \begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix}$$

$$\langle a_i|\hat{P}|a_j\rangle = \langle b_i|\hat{U}^+\hat{P}\hat{U}|b_j\rangle$$

or

$$\hat{U}^+\hat{P}\hat{U} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}\begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} 1+\varepsilon & 0 \\ 0 & 1-\varepsilon \end{pmatrix}$$

((**Mathematica**))

((Method A))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

A = {{1, ε}, {ε, 1}};
```

$$UT = \left\{\left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right\}\right\};$$

```
U = Transpose[UT]
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right\}\right\}$$

```
UH = UT*
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right\}\right\}$$

```
UH.A.U // Simplify

{{1 + ε, 0}, {0, 1 - ε}}
```

((Method B)). This problem can be also solved from a view point of eigenvalue problem.

```
Clear["Global`*"]

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]}

A = {{1, ε}, {ε, 1}};

eq1 = Eigensystem[A]

{{1 - ε, 1 + ε}, {{-1, 1}, {1, 1}}}
```

```
ψ1 = Normalize[eq1[[2, 1]]]
```

$$\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$$

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$$\left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$$

```
ψ1*.ψ2
```

0

```
UT = {ψ1, ψ2}
```

$$\left\{\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}\right\}$$

```
UH = UT*
```

$$\left\{\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}\right\}$$

```
UH // MatrixForm
```

$$\begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
U = Transpose[UT]
```

$$\left\{\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}\right\}$$

```
UH.U
```

{{1, 0}, {0, 1}}

```
UH.A.U // Simplify
```

$\{\{1 - \varepsilon, 0\}, \{0, 1 + \varepsilon\}\}$

4.28 Schaum 4-31, p.73 Non-degenerate case

Suppose that the energy of the system was measured and a value of E = 1 was found.

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}.$$

Subsequently we perform a measurement of a variable A described in the same basis by

$$\hat{A} = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 2 & i \\ 0 & -i & 2 \end{pmatrix}.$$

(a) Find the possible result of A. (b) What are the possibilities of obtaining each of the results found in part in (a)?

((**Soluition**))

(a) $a_1 = 1$, $a_2 = 3$, $a_3 = 5$
(b) P_1=1/4, P_2 = 1/4, and P_3 = 1/2

((**Mathematica**))

```
Clear["Global`*"]

exp_* := exp /. {Complex[re_, im_] :→ Complex[re, -im]}

A = {{5, 0, 0}, {0, 2, ⅈ}, {0, -ⅈ, 2}}
```

{{5, 0, 0}, {0, 2, ⅈ}, {0, -ⅈ, 2}}

```
A // MatrixForm
```

$$\begin{pmatrix} 5 & 0 & 0 \\ 0 & 2 & i \\ 0 & -i & 2 \end{pmatrix}$$

```
eq1 = Eigensystem[A]
```

{{5, 3, 1}, {{1, 0, 0}, {0, ⅈ, 1}, {0, -ⅈ, 1}}}

```
ψ1 = Normalize[eq1[[2, 1]]]
```

{1, 0, 0}

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$$\left\{0, \frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$\left\{0, -\frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$

```
φ = 1/√2 {1, -1, 0}
```

$\left\{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right\}$

```
Abs[ψ1*.φ]^2
```

$\frac{1}{2}$

```
Abs[ψ2*.φ]^2
```

$\frac{1}{4}$

```
Abs[ψ3*.φ]^2
```

$\frac{1}{4}$

4.29 Definition: degeneracy

Suppose that the eigenkets $\left|a_i\right\rangle$ (i = 1,2, …, ν) are the linearly independent eigenkets of $\hat{A}$ with the same eigenvalue:

$$\hat{A}\left|a_1\right\rangle = a\left|a_1\right\rangle, \qquad \hat{A}\left|a_2\right\rangle = a\left|a_2\right\rangle, \qquad \hat{A}\left|a_3\right\rangle = a\left|a_3\right\rangle, \ldots\ldots$$

where $\left\langle a_i \middle| a_j \right\rangle = \delta_{ij}$. Then the eigenvalue of these eigenkets is said to be degenerate

4.30 Griffiths; Problem 3-23 p.94 Degenerate case

Consider the following Hermitian matrix

$$\hat{A} = \begin{pmatrix} 2 & i & 1 \\ -i & 2 & i \\ 1 & -i & 2 \end{pmatrix}$$

(i) Calculate det($\hat{A}$) and Tr($\hat{A}$).

(ii) Find the eigenvalues of $\hat{A}$.
(iii) Find the eigenvectors of $\hat{A}$
(iv) Construct the Unitary matrix $\hat{U}$ that dioagonlizes $\hat{A}$.

((**Mathematica**))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] ⧴ Complex[re, -im]};
```

$$A = \begin{pmatrix} 2 & i & 1 \\ -i & 2 & i \\ 1 & -i & 2 \end{pmatrix};$$

```
{Det[A], Tr[A]}
```

{0, 6}

```
eq1 = Eigensystem[A]
```

{{3, 3, 0}, {{1, 0, 1}, {i, 1, 0}, {-1, -i, 1}}}

```
ψ1 = Normalize[eq1[[2, 1]]]
```

$$\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$$

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$$\left\{\frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}$$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$$\left\{-\frac{1}{\sqrt{3}}, -\frac{i}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}$$

```
{ψ1*.ψ2, ψ2*.ψ3, ψ3*.ψ1}
```

$$\left\{\frac{i}{2}, 0, 0\right\}$$

```
eq2 = Orthogonalize[{ψ1, ψ2}]
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{i}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{i}{\sqrt{6}}\right\}\right\}$$

We introduce a new eigenvector $\psi 21$ instead of $\psi 2$.

```
ψ21 = eq2[[2]]
```

$$\left\{\frac{i}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{i}{\sqrt{6}}\right\}$$

```
{ψ1*.ψ21, ψ21*.ψ3, ψ3*.ψ1}
```

{0, 0, 0}

```
UT = {ψ1, ψ21, ψ3}
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{i}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{i}{\sqrt{6}}\right\}, \left\{-\frac{1}{\sqrt{3}}, -\frac{i}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}\right\}$$

```
U = Transpose[UT]
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, \frac{i}{\sqrt{6}}, -\frac{1}{\sqrt{3}}\right\}, \left\{0, \sqrt{\frac{2}{3}}, -\frac{i}{\sqrt{3}}\right\}, \left\{\frac{1}{\sqrt{2}}, -\frac{i}{\sqrt{6}}, \frac{1}{\sqrt{3}}\right\}\right\}$$

```
UH = UT*
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{i}{\sqrt{6}}, \sqrt{\frac{2}{3}}, \frac{i}{\sqrt{6}}\right\}, \left\{-\frac{1}{\sqrt{3}}, \frac{i}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}\right\}$$

```
UH.U
```

{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

```
UH.A.U // Simplify
```

{{3, 0, 0}, {0, 3, 0}, {0, 0, 0}}

4.31 Schaum Problem 4-30, p.72 Degenerate case

Consider a physical system with a three dimensional system space. An orthnormal basis of the state space is chosen; in this basis the Hamiltonian is represented by the matrix,

$$\hat{H} = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}.$$

(a) What are the possible results when the energy of the system is measured? (b) A particle is in the state $|\psi\rangle$ represented in this basis as

$$|\psi\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} i \\ -i \\ i \end{pmatrix},$$

find $\langle\psi|\hat{H}|\psi\rangle$, $\langle\psi|\hat{H}^2|\psi\rangle$, and $\Delta H = \sqrt{\langle\psi|\hat{H}^2|\psi\rangle - \langle\psi|\hat{H}|\psi\rangle^2}$.

((**Solution**))

(a) $E_1 = 1$ and $E_2 = 3$. Note that E_1 is a nondegenerate eigenvalue, while E_2 is degenerate.

(b) $\langle\psi|\hat{H}|\psi\rangle$=5/3, $\langle\psi|\hat{H}^2|\psi\rangle$=11/3, and $\Delta H = 2\sqrt{2}/3$.

((**Mathematica**))

```
Clear["Global`*"]

exp_ * := exp /. {Complex[re_, im_] :> Complex[re, -im]}

H = {{2, 1, 0}, {1, 2, 0}, {0, 0, 3}}
```

{{2, 1, 0}, {1, 2, 0}, {0, 0, 3}}

```
H // MatrixForm
```

$$\begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$$

```
eq1 = Eigensystem[H]
```

{{3, 3, 1}, {{0, 0, 1}, {1, 1, 0}, {-1, 1, 0}}}

```
ψ1 = Normalize[eq1[[2, 1]]]
```

{0, 0, 1}

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$$\left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}$$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$$\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}$$

Orthogonality

```
{ψ1*.ψ2, ψ2*.ψ3, ψ3*.ψ1}
```

{0, 0, 0}

$$\psi = \frac{1}{\sqrt{3}}\{i, -i, i\}$$

$$\left\{\frac{i}{\sqrt{3}}, -\frac{i}{\sqrt{3}}, \frac{i}{\sqrt{3}}\right\}$$

```
ψ*.ψ
```

1

Average values

```
H1 = ψ*.H.ψ // Simplify
```

$$\frac{5}{3}$$

```
H2 = ψ*.H.H.ψ // Simplify
```

$$\frac{11}{3}$$

$$\Delta H = \sqrt{H2 - H1^2}$$

$$\frac{2\sqrt{2}}{3}$$

4.32 Shankar; Example 1.8.5, p.38 Degenerate case

Consider an Hermitian operator $\hat{A}$ given by

$$\hat{A} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix},$$

in the basis of $\{|b_1\rangle, |b_2\rangle, |b_3\rangle\}$. What are the eigenvalue a_i, and eigenvector $|a_i\rangle$?

((**Solution**))
We assume that

$$|a_i\rangle = \hat{U}|b_i\rangle,$$

where $\hat{U}$ is a unitary operator. Then the eigenvalue problem is as follows.

$$\hat{A}|a_i\rangle = a_i|a_i\rangle,$$

or

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = \lambda \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix},$$

or

$$\begin{pmatrix} 1-\lambda & 0 & 1 \\ 0 & 2-\lambda & 0 \\ 1 & 0 & 1-\lambda \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = 0.$$

The characteristic equation is given from the condition;

$$\begin{vmatrix} 1-\lambda & 0 & 1 \\ 0 & 2-\lambda & 0 \\ 1 & 0 & 1-\lambda \end{vmatrix} = 0, \text{ or } \lambda(\lambda-2)^2 = 0,$$

then we have

λ = 0, 2, and 2.

For λ = 0 (nondegenerate);

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = 0,$$

C_3 = -C_1, and C_2 = 0.

The normalization condition: $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$. Then we choose

$$C_1 = \frac{1}{\sqrt{2}},\ C_2 = 0,\ C_3 = -\frac{1}{\sqrt{2}}.$$

or

$$|\psi_{\lambda=0}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}.$$

For $\lambda = 2$ (degenerate case)

$$\begin{pmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = 0.$$

Then we have just one equation.

$$-C_1 + C_3 = 0.$$

This is a reflection of the degeneracy. Thus degeneracy permits us extra degree of freedom. The conditions

$$C_3 = C_1 \text{ and } C_2 \text{ (arbitrary).} \tag{1}$$

define an ensemble of eigenvectors that are orthogonal to $|\psi_{\lambda=0}\rangle$. Let us arbitrarily choose C_2 = 0. The first normalized eigenket for λ = 2 is

$$|\psi_{\lambda=2}, first\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}.$$

The second normalized eigenket for $\lambda = 2$ should be orthogonal to $\left|\psi_{\lambda=2}, first\right\rangle$.

$$\left|\psi_{\lambda=2}, \text{sec}ond\right\rangle = \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix},$$

$$\left\langle\psi_{\lambda=2}, first\middle|\psi_{\lambda=2}, \text{sec}ond\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = \frac{1}{\sqrt{2}}(C_1 + C_3) = 0,$$

or

$$C_3 = -C_1.$$

Uisng

$$C_3 = C_1,$$

from Eq.(1) and noting that $\left|C_1\right|^2 + \left|C_2\right|^2 + \left|C_3\right|^2 = 1$, we have $C_3 = C_1 = 0$ and C_2=1.

$$\left|\psi_{\lambda=2}, \text{sec}ond\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

In summary

$$\left|\psi_{\lambda=0}\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \qquad \left|\psi_{\lambda=2}, first\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \qquad \left|\psi_{\lambda=2}, \text{sec}ond\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

((**Mathematica**))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

A = (1 0 1
     0 2 0
     1 0 1);

eq1 = Eigensystem[A]
```

{{2, 2, 0}, {{1, 0, 1}, {0, 1, 0}, {-1, 0, 1}}}

```
ψ1 = Normalize[eq1[[2, 1]]]
```

$\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$

```
ψ2 = Normalize[eq1[[2, 2]]]
```

{0, 1, 0}

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$

```
{ψ1*.ψ2, ψ2*.ψ3, ψ3*.ψ1}
```

{0, 0, 0}

```
Orthogonalize[{ψ1, ψ2}]
```

$\left\{\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \{0, 1, 0\}\right\}$

```
UT = {ψ1, ψ2, ψ3}
```

$\left\{\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \{0, 1, 0\}, \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}\right\}$

```
U = Transpose[UT]
```

$\left\{\left\{\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right\}, \{0, 1, 0\}, \left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}\right\}$

```
UH = UT*
```

$\left\{\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \{0, 1, 0\}, \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}\right\}$

```
UH.U
```

{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

```
UH.A.U
```

{{2, 0, 0}, {0, 2, 0}, {0, 0, 0}}

4.33 Shankar; Exercise 1.8.3, p.41 Degenerate case

We consider the matrix of the Hermitian operator,

$$\hat{A} = \frac{1}{2}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & -1 \\ 0 & -1 & 3 \end{pmatrix}$$

(1) Show that the eigenvalues of $\hat{A}$ are given by $a_1 = a_2 = 1$, $a_3 = 2$.
(2) Find the eigenkets associated with $a_1 = a_2 = 1$, $a_3 = 2$.
(3) Find the unitary operator $\hat{U}$.
(4) Verify that $\hat{U}^+\hat{A}\hat{U}$ is diagonal.

The eigenvalue problem;

$$\frac{1}{2}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & -1 \\ 0 & -1 & 3 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = \lambda\begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix}$$

or

$$\begin{pmatrix} 1-\lambda & 0 & 0 \\ 0 & \frac{3}{2}-\lambda & -\frac{1}{2} \\ 0 & -\frac{1}{2} & \frac{3}{2}-\lambda \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = 0$$

The characteristic equation is given from the condition;

$$\begin{vmatrix} 1-\lambda & 0 & 0 \\ 0 & \frac{3}{2}-\lambda & -\frac{1}{2} \\ 0 & -\frac{1}{2} & \frac{3}{2}-\lambda \end{vmatrix} = 0 \text{ , or } (\lambda-2)(\lambda-1)^2 = 0$$

$\lambda = 2$, 1, and 1.

For $\lambda = 2$ (nondegenerate)

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{1}{2} \\ 0 & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = 0$$

$C_3 = -C_2$, and $C_1 = 0$.

The normalization condition: $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$.

Then we choose $C_2 = 1/\sqrt{2}$, $C_3 = -1/\sqrt{2}$, and $C_1 = 0$.

$$|\psi_{\lambda=2}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

For $\lambda = 1$ (degenerate)

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} \\ 0 & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = 0$$

Then we have just one equation.

$$C_2 = C_3$$

This is a reflection of the degeneracy. Thus degeneracy permits us extra degree of freedom. The conditions of

$$C_3 = C_2 \text{ and } C_1 \text{ (arbitrary).} \qquad (2)$$

define an ensemble of eigenvectors that are orthogonal to $|\psi_{\lambda=1}\rangle$.

Let us arbitrarily choose $C_1 = 0$. The first normalized eigenket for $\lambda = 1$ is

$$|\psi_{\lambda=1}, first\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

The second normalized eigenket for $\lambda = 1$ should be orthogonal to $|\psi_{\lambda=1}, first\rangle$.

$$|\psi_{\lambda=1}, \mathrm{sec}ond\rangle = \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix}$$

$$\langle\psi_{\lambda=1}, first|\psi_{\lambda=1}, \mathrm{sec}ond\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = \frac{1}{\sqrt{2}}(C_2 + C_3) = 0$$

or

$$C_3 = -C_2$$

$C_3 = C_2$ from Eq.(1). The normalization condition: $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$.
Then we have $C_3 = C_2 = 0$, and $C_1 = 1$,

$$|\psi_{\lambda=1}, \mathrm{sec}ond\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

In summary,

$$|\psi_{\lambda=2}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, \qquad |\psi_{\lambda=1}, first\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \qquad |\psi_{\lambda=1}, \mathrm{sec}ond\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

The unitary operator is obtained as

$$\hat{U} = \begin{pmatrix} 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \qquad \hat{U}^+ = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \end{pmatrix}$$

$$\hat{U}^{+}\hat{A}\hat{U} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
```

$$A = \frac{1}{2}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & -1 \\ 0 & -1 & 3 \end{pmatrix};$$

```
eq1 = Eigensystem[A]
```

{{2, 1, 1}, {{0, -1, 1}, {0, 1, 1}, {1, 0, 0}}}

```
ψ1 = Normalize[eq1[[2, 1]]]
```

$\left\{0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$\left\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

{1, 0, 0}

```
{ψ1*.ψ2, ψ2*.ψ3, ψ3*.ψ1}
```

{0, 0, 0}

```
Orthogonalize[{ψ2, ψ3}]
```

$\left\{\left\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \{1, 0, 0\}\right\}$

```
UT = {ψ1, ψ2, ψ3}
```

$\left\{\left\{0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \{1, 0, 0\}\right\}$

```
U = Transpose[UT]
```

$\left\{\{0, 0, 1\}, \left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}, \left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}\right\}$

```
UH = UT*
```

$\left\{\left\{0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \{1, 0, 0\}\right\}$

```
UH.U
```

{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

```
UH.A.U
```

{{2, 0, 0}, {0, 1, 0}, {0, 0, 1}}

4.34 Eigenvalue problems with subspace degenerate case

This method is sometimes very useful in understanding the concept of the eigenvalue problem. If you use the Mathematica, however, this problem is one of typical eigenvalue problems.

We consider the following Hermitian operator

$$\hat{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

under the basis of $\{|b_1\rangle, |b_2\rangle, |b_3\rangle\}$.

We need to find the eigenkets $|a_1\rangle, |a_2\rangle, |a_3\rangle$, where

$$\hat{A}|a_i\rangle = a_i|a_i\rangle$$

Before solving the eigenvalue problem, let us calculate

$$\hat{A}|b_1\rangle = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |b_1\rangle,$$

$$\hat{A}|b_2\rangle = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = |b_3\rangle,$$

$$\hat{A}|b_3\rangle = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = |b_2\rangle.$$

This means that $|a_1\rangle = |b_1\rangle$ is already an eigenket of $\hat{A}$ with the eigenvalue $a_1 = 1$.

$$|a_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

We now consider the subspace spanned by $\{|b_2\rangle, |b_3\rangle\}$. The restriction of $\hat{A}$ to the subspace is written as

$$\hat{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The eigenvalue problem is simplified as

$$\hat{A}|a_2\rangle = a_2|a_2\rangle, \qquad \hat{A}|a_3\rangle = a_3|a_3\rangle,$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \lambda\begin{pmatrix} C_1 \\ C_2 \end{pmatrix},$$

or

$$\begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0,$$

or

$$\lambda = \pm 1.$$

For $\lambda = 1$

$$\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0, \quad \text{or} \qquad C_1 = C_2,$$

$$|a_2\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|b_2\rangle + |b_3\rangle).$$

For $\lambda = -1$

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0, \qquad \text{or} \qquad C_1 = -C_2,$$

$$|a_3\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|b_2\rangle - |b_3\rangle).$$

In summary

$$|a_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |a_2\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \qquad |a_3\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}.$$

((**Mathematica**))

```
Clear["Global`*"];

exp_* :=
  exp /. {Complex[re_, im_] :> Complex[re, -im]};

A = (1 0 0
     0 0 1
     0 1 0);

eq1 = Eigensystem[A]

{{-1, 1, 1}, {{0, -1, 1}, {0, 1, 1}, {1, 0, 0}}}

ψ1 = Normalize[eq1[[2, 1]]]
```

$\left\{0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$\left\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$

```
ψ3 = Normalize[eq1[[2, 3]]]

{1, 0, 0}

{ψ1*. ψ2, ψ2* .ψ3 , ψ3* . ψ1}

{0, 0, 0}

UT = {ψ1, ψ2, ψ3};

U = Transpose[UT];

UH = ConjugateTranspose[U];

UH.A.U // Simplify

{{-1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

% // MatrixForm
```

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

4.35 Compatible observables and simultaneous measurement

((**Definition: compatible**))

Observables $\hat{A}$ and $\hat{B}$ are defined to be compatible when $[\hat{A},\hat{B}]=0$ and incompatible when $[\hat{A},\hat{B}]\neq 0$

We consider two Hermitian operators $\hat{A}$ and $\hat{B}$ that satisfy the relation, $[\hat{A},\hat{B}]=0$. Suppose the eigenvalue of these eigenkets of $\hat{A}$ is degenerate. For simplicity, we consider the case consisting of $|a_1\rangle$ and $|a_2\rangle$.

$$\hat{A}|a_1\rangle = a|a_1\rangle, \text{ and } \qquad \hat{A}|a_2\rangle = a|a_2\rangle,$$

or

$$\hat{A}=\begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}.$$

If we apply the operator $\hat{B}$ to this, we obtain

$$\hat{B}\hat{A}|a_1\rangle = a\hat{B}|a_1\rangle = \hat{A}\hat{B}|a_1\rangle,$$

$$\hat{B}\hat{A}|a_2\rangle = a\hat{B}|a_2\rangle = \hat{A}\hat{B}|a_2\rangle,$$

$\hat{B}|a_1\rangle$ and $\hat{B}|a_2\rangle$are also the eigenkest of $\hat{A}$ with the same eigenvalue *a*. Note that any combination of $|a_1\rangle$ and $|a_2\rangle$ is the eigenkest of $\hat{A}$ with the same eigenvalue *a*. Then $\hat{B}|a_i\rangle$ (i = 1, 2) can be described by

$$\hat{B}|a_1\rangle = b_{11}|a_1\rangle + b_{12}|a_2\rangle,$$

$$\hat{B}|a_2\rangle = b_{21}|a_1\rangle + b_{22}|a_2\rangle,$$

which means that the matrix $\hat{B}$ is not diagonal in the basis of $\{|a_i\rangle\}$.

$$\hat{B}=\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}.$$

Here we introduce the new kets $|\alpha_1\rangle$ and $|\alpha_2\rangle$ which are also the eigenket of $\hat{A}$.

$$|\alpha_1\rangle = \hat{U}|a_1\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = U_{11}|a_1\rangle + U_{21}|a_2\rangle,$$

and

$$|\alpha_2\rangle = \hat{U}|a_2\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix} = U_{12}|a_1\rangle + U_{22}|a_2\rangle,$$

where $\hat{U}$ is the unitary operator. We can solve the eigenvalue problem such that

$$\hat{B}|\alpha_1\rangle = b_1|\alpha_1\rangle \text{ and } \hat{B}|\alpha_2\rangle = b_2|\alpha_1\rangle.$$

In other words,

$$\hat{B}\hat{U}|a_1\rangle = b_1\hat{U}|a_1\rangle. \qquad \text{and} \qquad \hat{B}\hat{U}|a_2\rangle = b_2\hat{U}|a_2\rangle$$

or

$$\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = b_1\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}\begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix} = b_2\begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix}$$

Then we have

$$\hat{A}|\alpha_1\rangle = a|\alpha_1\rangle \text{ and } \hat{A}|\alpha_2\rangle = a|\alpha_1\rangle,$$

$$\hat{B}|\alpha_1\rangle = b_1|\alpha_1\rangle \text{ and } \hat{B}|\alpha_2\rangle = b_2|\alpha_1\rangle,$$

In other words, $|\alpha_1\rangle$ and $|\alpha_2\rangle$ are the simultaneous eigenkets of $\hat{A}$ and $\hat{B}$.

For convenience we introduce the new notation

$$|\alpha_1\rangle = |a, b_1\rangle \text{ and } |\alpha_2\rangle = |a, b_2\rangle.$$

The ket $|a,b\rangle$ ($b = b_1$, b_2) satisfies the relations,

$$\hat{A}|a,b\rangle = a|a,b\rangle, \qquad \hat{B}|a,b\rangle = b|a,b\rangle.$$

Then

$$\hat{A}\hat{B}|a,b\rangle = b\hat{A}|a,b\rangle = ab|a,b\rangle,$$

$$\hat{B}\hat{A}|a,b\rangle = a\hat{B}|a,b\rangle = ab|a,b\rangle,$$

or

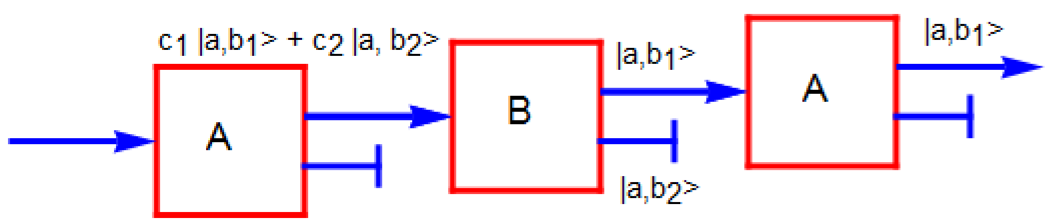
$$[\hat{A},\hat{B}]|a,b\rangle = 0,$$

or

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

In summary, the eigenket $|a,b\rangle$ is the simultaneous eigenket of $\hat{A}$ and $\hat{B}$.

We now consider the measurements of $\hat{A}$ and $\hat{B}$ when they are compatible. Suppose we measure $\hat{A}$ first and obtain result *a*. Subsequently we measure $\hat{B}$ and get result b_1. Finally we measure *A* again. It follows from our measurement formalism that third measurement always gives *a* with certainty, that is, the second (*B*) measurement does not destroy the previous information obtained in the first (*A*) measurement.



After the first (A) measurement, which yields *a*, the system is thrown into

$$c_1|a,b_1\rangle + c_2|a,b_2\rangle.$$

The second (B) measurement may select just one of the terms in the linear combination, say,

$$|a,b_1\rangle.$$

But the third (A) measurement applied to it still yields *a*. The state is described by

$$|a,b_1\rangle.$$

where $\hat{A}|a,b_1\rangle = a|a,b_1\rangle$ and $\hat{B}|a,b_1\rangle = b_1|a,b_1\rangle$. The *A* and *B* measurements do not interfere.

4.36 Incompatible observables

We have seen that only commuting observables can in principle be measured and specified with perfect precision simultaneously. If $\hat{A}$ and $\hat{B}$ are two Hermitian operators that do not commute, the physical quantities *A* and *B* cannot both be sharply defined simultaneously. This suggests that the degree to which the commutator $[\hat{A},\hat{B}]$ of $\hat{A}$ and $\hat{B}$ is different from zero may give us information about the inevitable lack of precision in simultaneously specifying both of these observables.

((Note))

$$[\hat{x},\hat{p}] = i\hbar .$$

These two quantities can never be defined simultaneously with infinite precision.

For a given system, the measurement of *A* followed by the measurement of *B* is denoted by $\hat{B}\hat{A}$, and the result may be different for $\hat{A}\hat{B}$. If the measurement interfere with each other, then the commutator $[\hat{A},\hat{B}]$. When $[\hat{A},\hat{B}] = 0$, the measurements do not interfere with each other.

4.37 Sakurai 1-23, p.65 Simultaneous eigenvectors

Consider a three-dimensional ket space. If a certain set of orthonormal kets-say, $|1\rangle,|2\rangle,|3\rangle$ - are used as the base kets, the operators $\hat{A}$ and $\hat{B}$ are represented by

$$\hat{A} = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}, \qquad \hat{B} = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix},$$

with *a* and *b* are both real.

or

a. Obviously, $\hat{A}$ exhibits a degenerate spectrum. Does $\hat{B}$ also exhibit a degenerate spectrum?
b. Show that $\hat{A}$ and $\hat{B}$ commute.
c. Find a new set of orthonormal kets which are simultaneous eigenkets of both $\hat{A}$ and $\hat{B}$. Specify the eigenvalues of $\hat{A}$ and $\hat{B}$ for each of the three eigenkets. Does your specification of eigenvalues completely characterize each eigenket?

((**Solution**))

$\hat{A}|1\rangle = a|1\rangle$, $\hat{A}|2\rangle = -a|2\rangle$, $\hat{A}|3\rangle = -a|3\rangle$,

$\hat{B}|1\rangle = b|1\rangle$, $\hat{B}|2\rangle = ib|3\rangle$, $\hat{B}|3\rangle = -ib|2\rangle$,

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

The eigenkets of $\hat{B}$ should be the eigenkets of $\hat{A}$, and vice versa.
The operators $\hat{A}$ and $\hat{B}$ are the Hermitian operators.

Eigenkets of $\hat{A}$:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \text{(eigenvalue: } a\text{)}$$

$$|2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{(eigenvalue: -}a\text{)}$$

$$|3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \qquad \text{(eigenvalue: -}a\text{)}$$

Any combination of $|2\rangle$ and $|3\rangle$ is the eigenket of $\hat{A}$ with the eigenvalue (-*a*).

Eigenkets of $\hat{B}$:

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |1\rangle, \qquad \text{(eigenvalue: } b\text{)}$$

$\hat{B}|2\rangle = ib|3\rangle$, $\hat{B}|3\rangle = -ib|2\rangle$.

In the subspace spanned by $|2\rangle$ and $|3\rangle$, we consider the eigenvalue problem

$$\hat{B}_{sub} = \begin{pmatrix} 0 & -ib \\ ib & 0 \end{pmatrix},$$

$$\hat{B}_{sub}|\phi\rangle = \lambda|\phi\rangle,$$

with

$$|\phi\rangle = \begin{pmatrix} C_2 \\ C_3 \end{pmatrix},$$

$$\begin{pmatrix} 0 & -ib \\ ib & 0 \end{pmatrix}\begin{pmatrix} C_2 \\ C_3 \end{pmatrix} = \lambda\begin{pmatrix} C_2 \\ C_3 \end{pmatrix},$$

or

$$\begin{pmatrix} -\lambda & -ib \\ ib & -\lambda \end{pmatrix}\begin{pmatrix} C_2 \\ C_3 \end{pmatrix} = 0,$$

$$M = \begin{pmatrix} -\lambda & -ib \\ ib & -\lambda \end{pmatrix}.$$

Det[M]=0:

$$\begin{vmatrix} -\lambda & -ib \\ ib & -\lambda \end{vmatrix} = \lambda^2 - b^2 = 0, \qquad \text{or } \lambda = \pm b.$$

(i) $\lambda = b$

$$\begin{pmatrix} -b & -ib \\ ib & -b \end{pmatrix}\begin{pmatrix} C_2 \\ C_3 \end{pmatrix} = 0,$$

$$C_3 = iC_2,$$

$$|C_2|^2 + |C_3|^3 = 1.$$

Then we have $C_2 = -\dfrac{i}{\sqrt{2}}$ and $C_3 = \dfrac{1}{\sqrt{2}}$,

or

$$|\psi_2\rangle = \begin{pmatrix} 0 \\ -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = -\frac{i}{\sqrt{2}}|2\rangle + \frac{1}{\sqrt{2}}|3\rangle: \quad \text{(eigenvalue } b\text{)}.$$

(ii) $\lambda = -b$

$$\begin{pmatrix} b & -ib \\ ib & b \end{pmatrix}\begin{pmatrix} C_2 \\ C_3 \end{pmatrix} = 0,$$

$$C_3 = iC_2,$$

$$|C_2|^2 + |C_3|^3 = 1.$$

Then we have $C_2 = -\frac{i}{\sqrt{2}}$ and $C_3 = \frac{1}{\sqrt{2}}$.

or

$$|\psi_3\rangle = \begin{pmatrix} 0 \\ \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{i}{\sqrt{2}}|2\rangle + \frac{1}{\sqrt{2}}|3\rangle: \qquad \text{(eigenvalue } -b\text{)}$$

Since any combinations of $|2\rangle$ and $|3\rangle$ are the eigenkets of $\hat{A}$ with an eigenvalue (-*a*). Then

$$\hat{A}|\psi_2\rangle = -a|\psi_2\rangle, \qquad \text{and} \qquad \hat{A}|\psi_3\rangle = -a|\psi_3\rangle$$

In conclusion, $|\psi_1\rangle$, $|\psi_2\rangle$, and $|\psi_3\rangle$ are the simultaneous eigenkets of $\hat{A}$ and $\hat{B}$.

((**Mathematica**))

```
A = ( a  0   0
      0 -a   0
      0  0  -a );
B = ( b  0    0
      0  0  -ⅈ b
      0 ⅈ b   0 );
```

(a)

```
eq1 = Eigensystem[A]
```

```
{{-a, -a, a}, {{0, 0, 1}, {0, 1, 0}, {1, 0, 0}}}
```

```
ψa1 = Normalize[eq1[[2, 1]]]
```

```
{0, 0, 1}
```

```
ψa2 = Normalize[eq1[[2, 2]]]
```

```
{0, 1, 0}
```

```
ψa3 = Normalize[eq1[[2, 3]]]
```

```
{1, 0, 0}
```

```
{ψa1*.ψa2, ψa2*.ψa3, ψa3*.ψa1}
```

```
{0, 0, 0}
```

```
Orthogonalize[{ψa1, ψa2}]
```

```
{{0, 0, 1}, {0, 1, 0}}
```

Any combination of ψa1 and ψa2 belongs to the eigenvalue of A with the eigenvalue (-a)

```
eq2 = Eigensystem[B]
```

{{-b, b, b}, {{0, i, 1}, {0, -i, 1}, {1, 0, 0}}}

{{-b, b, b}, {{0, i, 1}, {0, -i, 1}, {1, 0, 0}}}

```
ψb1 = Normalize[eq2[[2, 1]]]
```

$$\left\{0, \frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$$

$$\left\{0, \frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$$

```
ψb2 = Normalize[eq2[[2, 2]]]
```

$$\left\{0, -\frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$$

$$\left\{0, -\frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$$

```
ψb3 = Normalize[eq2[[2, 3]]]
```

{1, 0, 0}

```
{ψb1*.ψb2, ψb2*.ψb3, ψb3*.ψb1}
```

{0, 0, 0}

(b)

```
A.B - B.A // Simplify
```

{{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}

(c) The simultaneous eigenvectors of A and B

Summary

$\psi b1 = \frac{-i}{\sqrt{2}} \psi a2 + \frac{1}{\sqrt{2}} \psi a1$ (A : -a, B : -b)

$\psi b2 = \frac{i}{\sqrt{2}} \psi a2 + \frac{1}{\sqrt{2}} \psi a1$ (A, -a, B : b)

$\psi b3 = \psi a3$ (A : a, B : b)

```
UT = {ψb1, ψb2, ψb3}
```

$\left\{\left\{0, \frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{0, -\frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \{1, 0, 0\}\right\}$

```
U = Transpose[UT]
```

$\left\{\{0, 0, 1\}, \left\{\frac{i}{\sqrt{2}}, -\frac{i}{\sqrt{2}}, 0\right\}, \left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}\right\}$

```
UH = UT*
```

$\left\{\left\{0, -\frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{0, \frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \{1, 0, 0\}\right\}$

```
UH.A.U
```

{{-a, 0, 0}, {0, -a, 0}, {0, 0, a}}

```
UH.B.U
```

{{-b, 0, 0}, {0, b, 0}, {0, 0, b}}

4.38 Tannoudji; Problem11, p.206 Simultaneous eigenvectors

Consider a physical system whose 3D state space is spanned by the orthonormal basis formed by the three kets -say, $|1\rangle, |2\rangle, |3\rangle$. In the basis of these three vectors, taken in this order, the two operators $\hat{A}$ and $\hat{B}$ are represented by

$$\hat{A} = \begin{pmatrix} E_0 & 0 & 0 \\ 0 & -E_0 & 0 \\ 0 & 0 & -E_0 \end{pmatrix}, \qquad \hat{B} = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & b \\ 0 & b & 0 \end{pmatrix}$$

where E_0 and b are constants.

(a) Are $\hat{A}$ and $\hat{B}$ Hermitian?

(b) Show that $\hat{A}$ and $\hat{B}$ commute. Give a basis of eigenvectors common to $\hat{A}$ and $\hat{B}$.

$$\hat{A}|1\rangle = E_0|1\rangle, \quad \hat{A}|2\rangle = -E_0|2\rangle, \qquad \hat{A}|3\rangle = -E_0|3\rangle,$$

$$\hat{B}|1\rangle = b|1\rangle, \quad \hat{B}|2\rangle = b|3\rangle \qquad \hat{B}|3\rangle = b|2\rangle,$$

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

Eigenkets of $\hat{A}$:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \text{(eigenvalue: } E_0\text{)}$$

$$|2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{(eigenvalue: - } E_0\text{)}$$

$$|3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \qquad \text{(eigenvalue: - } E_0\text{)}$$

Any combination of $|2\rangle$and $|3\rangle$ is the eigenket of $\hat{A}$ with the eigenvalue (-E_0).

Eigenkets of $\hat{B}$:

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |1\rangle, \qquad \text{(eigenvalue: } b\text{)}$$

In the subspace spanned by $|2\rangle$ and $|3\rangle$, we consider the eigenvalue problem

$$\hat{B}_{sub} = \begin{pmatrix} 0 & b \\ b & 0 \end{pmatrix},$$

$$\hat{B}_{sub}|\phi\rangle = \lambda|\phi\rangle,$$

with

$$|\phi_2\rangle = \hat{U}|2\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix},$$

$$|\phi_3\rangle = \hat{U}|3\rangle = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix}$$
$$= \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix}.$$

Eigenvalue problem

$$\begin{pmatrix} 0 & b \\ b & 0 \end{pmatrix}\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \lambda\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix},$$

or

$$\begin{pmatrix} -\lambda & b \\ b & -\lambda \end{pmatrix}\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = 0,$$

$$M = \begin{pmatrix} -\lambda & b \\ b & -\lambda \end{pmatrix}.$$

Det[M]=0:

$$\begin{vmatrix} -\lambda & b \\ b & -\lambda \end{vmatrix} = \lambda^2 - b^2 = 0, \qquad \text{or } \lambda = \pm b.$$

(i) $\lambda = b$

$$\begin{pmatrix} -b & b \\ b & -b \end{pmatrix}\begin{pmatrix} C_2 \\ C_3 \end{pmatrix} = 0,$$

$$C_3 = C_2,$$

$$|C_2|^2 + |C_3|^3 = 1.$$

Then we have $C_2 = C_3 = \dfrac{1}{\sqrt{2}}$,

or

$$|\psi_2\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|2\rangle + |3\rangle)$$: (eigenvalue b).

(ii) λ = -b

$$\begin{pmatrix} b & b \\ b & b \end{pmatrix}\begin{pmatrix} C_2 \\ C_3 \end{pmatrix} = 0,$$

$$C_3 = -C_2,$$

$$|C_2|^2 + |C_3|^3 = 1$$

Then we have $C_2 = \frac{1}{\sqrt{2}}$ and $C_3 = -\frac{1}{\sqrt{2}}$,

or

$$|\psi_3\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|2\rangle - |3\rangle):$$ (eigenvalue -b).

Since any combinations of $|2\rangle$ and $|3\rangle$ are the eigenkets of $\hat{A}$ with an eigenvalue (-a). Then

$$\hat{A}|\psi_2\rangle = -E_0|\psi_2\rangle, \qquad \text{and} \qquad \hat{A}|\psi_3\rangle = -E_0|\psi_3\rangle.$$

In conclusion, $|\psi_1\rangle$, $|\psi_2\rangle$, and $|\psi_3\rangle$ are the simultaneous eigenkets of $\hat{A}$ and $\hat{B}$.

((Mathematica))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]}

A = ( E0   0    0
      0   -E0   0
      0    0   -E0 );

B = ( b 0 0
      0 0 b
      0 b 0 );
```

(b)

```
A.B - B.A // Simplify

{{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}

eq1 = Eigensystem[A]

{{-E0, -E0, E0}, {{0, 0, 1}, {0, 1, 0}, {1, 0, 0}}}

ψa1 = Normalize[eq1[[2, 1]]]

{0, 0, 1}

ψa2 = Normalize[eq1[[2, 2]]]

{0, 1, 0}

ψa3 = Normalize[eq1[[2, 3]]]

{1, 0, 0}
```

```
eq2 = Eigensystem[B]
```

{{-b, b, b}, {{0, -1, 1}, {0, 1, 1}, {1, 0, 0}}}

```
ψb1 = Normalize[eq2[[2, 1]]]
```

$\{0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$

```
ψb2 = Normalize[eq2[[2, 2]]]
```

$\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$

```
ψb3 = Normalize[eq2[[2, 3]]]
```

{1, 0, 0}

```
{ψb1*.ψb2, ψb2*.ψb3, ψb3*.ψb1}
```

{0, 0, 0}

$\psi b1 = \frac{-1}{\sqrt{2}}\psi a2 + \frac{1}{\sqrt{2}}\psi a1$ (A : -E0, B : -b)

$\psi b2 = \frac{1}{\sqrt{2}}\psi a2 + \frac{1}{\sqrt{2}}\psi a1$ (A, -E0, B : b)

$\psi b3 = \psi a3$ (A : E0, B : b)

4.39 Shankar; Exercise 1.8.10, p.46 Simultaneous eigenvectors

By considering the commutator, show that the following Hermitian matrices may be simultaneously diagonized. Find the eigenvectors common to both and verify that under a unitary transformation to this basis, both matrices are diagonalized.

$$\hat{A} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \qquad \hat{B} = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{pmatrix}$$

((**Solution**))

We use the Mathematica to calculate the eigenvalues and eigenvectors of $\hat{A}$ and $\hat{B}$.

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

Using the Mathematica;

Eigensystem[$\hat{A}$],

we have the following results.

(a) $\lambda = 2$ (nondegenerate)

$$|\alpha_{\lambda=2}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix},$$

(b) $\lambda = 0$ (degenerate)

$$|\alpha_{\lambda=0}(1)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \qquad |\alpha_{\lambda=0}(2)\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

Here note that $|\alpha_{\lambda=2}\rangle$, $|\alpha_{\lambda=0}(1)\rangle$, and $|\alpha_{\lambda=0}(2)\rangle$ are orthogonal to each other. Any linear combination of $|\alpha_{\lambda=0}(1)\rangle$ and $|\alpha_{\lambda=0}(2)\rangle$ belong to the eigenvalue $\lambda = 0$ of $\hat{A}$.

Using the Mathematica;

Eigensystem[$\hat{B}$],

we have the following results.

(c) $\lambda = 3$ (nondegenerate)

$$|\beta_{\lambda=3}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}.$$

(d) $\lambda = 2$ (nondegenerate)

$$|\beta_{\lambda=2})\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}.$$

(e) λ = -1 (nondegenerate)

$$\left|\beta_{\lambda=-1}(2)\right\rangle = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ -2 \\ -1 \end{pmatrix}.$$

$\left|\beta_{\lambda=3}\right\rangle$, $\left|\beta_{\lambda=2}1)\right\rangle$, and $\left|\beta_{\lambda=-1})\right\rangle$ are orthogonal to each other. Thus we have the simultaneous eigen kets of $\hat{A}$ and $\hat{B}$

(1)

$$\left|\psi_1\right\rangle = \left|\beta_{\lambda=3}\right\rangle = \left|\alpha_{\lambda=2}\right\rangle,$$

with

$$\hat{A}\left|\psi_1\right\rangle = 2\left|\psi_1\right\rangle \text{ and } \hat{B}\left|\psi_1\right\rangle = 3\left|\psi_1\right\rangle.$$

(2)

$$\left|\psi_2\right\rangle = \left|\beta_{\lambda=2}\right\rangle = \frac{1}{\sqrt{3}}(\sqrt{2}\left|\alpha_{\lambda=0}(1)\right\rangle + \left|\alpha_{\lambda=0}(2)\right\rangle,$$

with

$$\hat{A}\left|\psi_2\right\rangle = 0\left|\psi_2\right\rangle \text{ and } \hat{B}\left|\psi_2\right\rangle = 2\left|\psi_2\right\rangle,$$

with

(3)

$$\left|\psi_3\right\rangle = \left|\beta_{\lambda=-1}\right\rangle = \frac{1}{\sqrt{3}}(\left|\alpha_{\lambda=0}(1)\right\rangle - \sqrt{2}\left|\alpha_{\lambda=0}(2)\right\rangle,$$

with

$$\hat{A}\left|\psi_3\right\rangle = 0\left|\psi_3\right\rangle \text{ and } \hat{B}\left|\psi_3\right\rangle = -\left|\psi_3\right\rangle.$$

Unitary operator is given by

$$\hat{U} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} \end{pmatrix}$$

$$\hat{U}^{+}\hat{A}\hat{U} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\hat{U}^{+}\hat{B}\hat{U} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"];

exp_ * := exp /. {Complex[re_, im_] :> Complex[re, -im]}

A = {{1, 0, 1}, {0, 0, 0}, {1, 0, 1}};

B = {{2, 1, 1}, {1, 0, -1}, {1, -1, 2}};
```

(a)

```
A.B - B.A // Simplify
```

{{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}

```
eq1 = Eigensystem[A]
```

{{2, 0, 0}, {{1, 0, 1}, {-1, 0, 1}, {0, 1, 0}}}

```
ψa1 = Normalize[eq1[[2, 1]]]
```

$\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$

```
ψa2 = Normalize[eq1[[2, 2]]]
```

$\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$

```
ψa3 = Normalize[eq1[[2, 3]]]
```

{0, 1, 0}

```
{ψa1*.ψa2, ψa2*.ψa3, ψa3*.ψa1}
```

{0, 0, 0}

```
eq2 = Eigensystem[B]
{{3, 2, -1}, {{1, 0, 1}, {-1, -1, 1}, {-1, 2, 1}}}
```

ψb1 = Normalize[eq2[[2, 1]]]

$$\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$$

ψb2 = Normalize[eq2[[2, 2]]]

$$\left\{-\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}$$

ψb3 = Normalize[eq2[[2, 3]]]

$$\left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, \frac{1}{\sqrt{6}}\right\}$$

{ψb1*.ψb2, ψb2*.ψb3, ψb3*.ψb1}

{0, 0, 0}

Summary

$\psi a1 = \psi b1 = \left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$ (A: eigenvalue 2, B: eigenvalue 3)

$\psi a2 = \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$ (A: 0), $\psi b2 = \left\{-\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}$ (B; 2)

$\psi a3=\{0, 1, 0\}$ (A: 0), $\psi b3 = \left\{-\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}$ (B: -1)

Note that

$\psi b2 = \frac{1}{\sqrt{3}}\left(\sqrt{2}\ \psi a2 + \psi a3\right), \psi b3 = \frac{1}{\sqrt{3}}\left(\sqrt{2}\ \psi a2 - \psi a3\right)$ are the eigenvectors of A with the eigenvalue 0 since any combination of $\psi a2$ and $\psi a3$ is an eigenvector of A with the eigenvalue 0.

```
UT = {ψb1, ψb2, ψb3}
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, \frac{1}{\sqrt{6}}\right\}\right\}$$

```
U = Transpose[UT]
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{6}}\right\}, \left\{0, -\frac{1}{\sqrt{3}}, \sqrt{\frac{2}{3}}\right\}, \left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{6}}\right\}\right\}$$

```
UH = UT*
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, \frac{1}{\sqrt{6}}\right\}\right\}$$

```
UH.U
{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

UH.A.U
{{2, 0, 0}, {0, 0, 0}, {0, 0, 0}}

UH.B.U // Simplify
{{3, 0, 0}, {0, 2, 0}, {0, 0, -1}}
```

APPENDIX: Elementary matrix properties (Mathematica)

1. **Tr[** $\hat{A}$ **]** To finds the trace of the matrix or tensor.
The trace of the matrix $\hat{A}$ is the sum over its diagonal elements.

$$Tr(\hat{A}) = \sum_k A_{kk}$$

2. **Transpose[** $\hat{A}$ **]** To give the usual transpose of a matrix $\hat{A}$.
The transpose of the matrix $\hat{A}$ is written as $\hat{A}^T$. The matrix elements of $\hat{A}^T$ $\hat{A}^T$ are obtained by reflecting the elements A_{nm} through the major diagonal of the matrix of $\hat{A}$.

3. **Inverse[** $\hat{A}$ **]** To give the inverse of a square matrix $\hat{A}$.

The inverse of the matrix $\hat{A}$ is labeled as $\hat{A}^{-1}$. It has the property that

$$\hat{A}\hat{A}^{-1} = \hat{A}^{-1}\hat{A} = \hat{1}$$

4. **Det[$\hat{A}$]** To give the determinant of the square matrix $\hat{A}$.

5. **HermitianMatrixQ[$\hat{A}$]** To test whether $\hat{A}$ is a Hermitian matrix.

6. **ConjugateTranspose[$\hat{A}$]** To give the conjugate transpose of $\hat{A}$.

7. **Orhogonalize[v_1, v_2,...]** To gives an orthonormal basis found by orthogonalizing the vectors {$\boldsymbol{v}_1$, v_2, …}.

8. **IdentityMatrix[n]** For the identity matrix of n x n.

The matrix element of the identity matrix $\hat{1}$ (or I) is given by the Kronecker delta.

$$\hat{1} = \begin{pmatrix} 1 & 0 & 0 & . & . & 0 \\ 0 & 1 & 0 & . & . & 0 \\ 0 & 0 & 1 & . & . & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{pmatrix}$$

8. **DiagonalMatrix[{g_1, g_2, g_3, …..}]** to make a diagonal matrix.

The matrix is given by

$$G_{nm} = g_n \delta_{nm}$$

$$\hat{G} = \begin{pmatrix} g_1 & 0 & 0 & . & . & 0 \\ 0 & g_2 & 0 & . & . & 0 \\ 0 & 0 & g_3 & . & . & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{pmatrix}$$

```
DiagonalMatrix[{1, 2, 3, 4}]
```

```
{{1, 0, 0, 0}, {0, 2, 0, 0}, {0, 0, 3, 0}, {0, 0, 0, 4}}
```

```
% // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix}$$

9. **UnitVector[n, k]** To give the n-dimensional unit vector in the k\[Null]th direction

```
UnitVector[5, 1]
```

```
{1, 0, 0, 0, 0}
```

```
UnitVector[5, 4]
```

```
{0, 0, 0, 1, 0}
```

10. **Outer[Times, ψ, φ^*]** To give an outer product of $|\psi\rangle\langle\varphi|$

$|\psi\rangle = \{a_1, a_2, a_3\}$; $\langle\varphi| = \{b_1^*, b_2^*, b_3^*\}$

```
ψ = {a1, a2, a3}; ϕ = {b1cc, b2cc, b3cc};
```

```
Outer[Times, ψ, ϕ]
```

```
{{a1 b1cc, a1 b2cc, a1 b3cc},
 {a2 b1cc, a2 b2cc, a2 b3cc}, {a3 b1cc, a3 b2cc, a3 b3cc}}
```

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APPENDIX

We solve the eigenvalue problems of problems in Chapter 3 of the book written byArfken and Weber book.

A.1 Arfken 3-5-21 non-degenerate case

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
```

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix};$$

```
eq1 = Eigensystem[A]
```

$$\left\{\left\{-\sqrt{2}, \sqrt{2}, 0\right\}, \left\{\left\{1, -\sqrt{2}, 1\right\}, \left\{1, \sqrt{2}, 1\right\}, \{-1, 0, 1\}\right\}\right\}$$

```
ψ1 = Normalize[eq1[[2, 1]]]
```

$$\left\{\frac{1}{2}, -\frac{1}{\sqrt{2}}, \frac{1}{2}\right\}$$

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$$\left\{\frac{1}{2}, \frac{1}{\sqrt{2}}, \frac{1}{2}\right\}$$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$$\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$$

```
{ψ1*.ψ2, ψ2*.ψ3, ψ3*.ψ1}
```

$\{0, 0, 0\}$

```
UT = {ψ1, ψ2, ψ3}
```

$\left\{\left\{\frac{1}{2}, -\frac{1}{\sqrt{2}}, \frac{1}{2}\right\}, \left\{\frac{1}{2}, \frac{1}{\sqrt{2}}, \frac{1}{2}\right\}, \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}\right\}$

```
U = Transpose[UT]
```

$\left\{\left\{\frac{1}{2}, \frac{1}{2}, -\frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}, \left\{\frac{1}{2}, \frac{1}{2}, \frac{1}{\sqrt{2}}\right\}\right\}$

```
UH = UT*
```

$\left\{\left\{\frac{1}{2}, -\frac{1}{\sqrt{2}}, \frac{1}{2}\right\}, \left\{\frac{1}{2}, \frac{1}{\sqrt{2}}, \frac{1}{2}\right\}, \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}\right\}$

```
UH.U
```

$\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$

```
UH.A.U // Simplify
```

$\left\{\left\{-\sqrt{2}, 0, 0\right\}, \left\{0, \sqrt{2}, 0\right\}, \{0, 0, 0\}\right\}$

```
% // MatrixForm
```

$$\begin{pmatrix} -\sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

A.2 Arfken 3-5-23 non-degenerate case

$$A = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

((Mathematica))

```
Clear["Global`*"];

exp_* :=
  exp /.
   {Complex[re_, im_] :> Complex[re, -im]};

A = (2 0 0
     0 1 1
     0 1 1);

eq1 = Eigensystem[A]

{{2, 2, 0},
 {{0, 1, 1}, {1, 0, 0}, {0, -1, 1}}}

ψ1 = Normalize[eq1[[2, 1]]]
```

$\left\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$

```
ψ2 = Normalize[eq1[[2, 2]]]

{1, 0, 0}

ψ3 = Normalize[eq1[[2, 3]]]
```

$\left\{0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$

```
{ψ1*.ψ2, ψ2*.ψ3, ψ3*.ψ1}
```

$\{0, 0, 0\}$

```
UT = {ψ1, ψ2, ψ3}
```

$$\left\{\left\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \{1, 0, 0\}, \left\{0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}\right\}$$

```
U = Transpose[UT]
```

$$\left\{\{0, 1, 0\}, \left\{\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right\}, \left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}\right\}$$

```
UH = UT*
```

$$\left\{\left\{0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \{1, 0, 0\}, \left\{0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}\right\}$$

```
UH.U
```

$\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$

```
UH.A.U // Simplify
```

$\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 0\}\}$

```
% // MatrixForm
```

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

A.3 Arfken 3-5-24 degenerate case

$$A = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"];

exp_* :=
  exp /.
   {Complex[re_, im_] :> Complex[re, -im]};
```

$$A = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix};$$

```
eq1 = Eigensystem[A]
```

{{2, -1, -1},
 {{1, 1, 1}, {-1, 0, 1}, {-1, 1, 0}}}

```
ψ1 = Normalize[eq1[[2, 1]]]
```

$$\left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}$$

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$$\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$$\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}$$

```
{ψ1*.ψ2, ψ2*.ψ3, ψ3*.ψ1}
```

$$\left\{0, \frac{1}{2}, 0\right\}$$

```
eq2 = Orthogonalize[{ψ2, ψ3}]
```

$$\left\{\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}\right\}$$

```
ψ31 = eq2[[2]]
```

$$\left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}$$

```
UT = {ψ1, ψ2, ψ31}
```

$$\left\{\left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}\right\}$$

```
U = Transpose[UT]
```

$$\left\{\left\{\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{6}}\right\}, \left\{\frac{1}{\sqrt{3}}, 0, \sqrt{\frac{2}{3}}\right\}, \left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{6}}\right\}\right\}$$

```
UH = UT*
```

$$\left\{\left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}\right\}$$

```
UH.U
```

{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

```
UH.A.U // Simplify
```

{{2, 0, 0}, {0, -1, 0}, {0, 0, -1}}

```
% // MatrixForm
```

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

A.4 Arfken 3-5-25 degenerate case

$$A = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"];

exp_* :=
  exp /.
   {Complex[re_, im_] :> Complex[re, -im]};
```

$$A = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix};$$

```
eq1 = Eigensystem[A]
```

```
{{2, 2, -1},
 {{-1, 0, 1}, {-1, 1, 0}, {1, 1, 1}}}
```

```
ψ1 = Normalize[eq1[[2, 1]]]
```

$$\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$$

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$$\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}$$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$$\left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}$$

$$\{\psi 1^{*}.\psi 2,\ \psi 2^{*}.\psi 3,\ \psi 3^{*}.\psi 1\}$$

$$\left\{\frac{1}{2}, 0, 0\right\}$$

```
eq2 = Orthogonalize[{ψ1, ψ2}]
```

$$\left\{\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}\right\}$$

```
ψ21 = eq2[[2]]
```

$$\left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}$$

```
UT = {ψ1, ψ21, ψ3}
```

$$\left\{\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}, \left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}\right\}$$

```
U = Transpose[UT]
```

$$\left\{\left\{-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{6}}, \frac{1}{\sqrt{3}}\right\}, \left\{0, \sqrt{\frac{2}{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{6}}, \frac{1}{\sqrt{3}}\right\}\right\}$$

```
UH = UT*
```

$$\left\{\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}, \left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}\right\}$$

```
UH.U
```

{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

```
UH.A.U
```

{{2, 0, 0}, {0, 2, 0}, {0, 0, -1}}

```
% // MatrixForm
```

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

A.5 Arfken 3-5-26 degenerate case

$$A = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"];

exp_* :=
  exp /.
   {Complex[re_, im_] :> Complex[re, -im]};
```

$$A = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix};$$

```
eq1 = Eigensystem[A]
```

```
{{2, -1, -1},
 {{1, 1, 1}, {-1, 0, 1}, {-1, 1, 0}}}
```

```
ψ1 = Normalize[eq1[[2, 1]]]
```

$$\left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}$$

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$$\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$$\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}$$

$$\{\psi 1^{*}.\psi 2,\ \psi 2^{*}.\psi 3,\ \psi 3^{*}.\psi 1\}$$

$$\left\{0, \frac{1}{2}, 0\right\}$$

```
eq2 = Orthogonalize[{ψ2, ψ3}]
```

$$\left\{\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}\right\}$$

```
ψ31 = eq2[[2]]
```

$$\left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}$$

```
UT = {ψ1, ψ2, ψ31}
```

$$\left\{\left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}\right\}$$

```
U = Transpose[UT]
```

$$\left\{\left\{\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{6}}\right\}, \left\{\frac{1}{\sqrt{3}}, 0, \sqrt{\frac{2}{3}}\right\}, \left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{6}}\right\}\right\}$$

```
UH = UT*
```

$$\left\{\left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}\right\}$$

```
UH.U
```

{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

```
UH.A.U // Simplify
```

{{2, 0, 0}, {0, -1, 0}, {0, 0, -1}}

```
% // MatrixForm
```

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

A.6 Arfken 3-5-28 degenerate case

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

A = (1 1 0
     1 1 0
     0 0 0);

eq1 = Eigensystem[A]

{{2, 0, 0}, {{1, 1, 0}, {0, 0, 1}, {-1, 1, 0}}}

ψ1 = Normalize[eq1[[2, 1]]]
```

$\left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}$

```
ψ2 = Normalize[eq1[[2, 2]]]

{0, 0, 1}

ψ3 = Normalize[eq1[[2, 3]]]
```

$\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}$

```
{ψ1*.ψ2, ψ2*.ψ3, ψ3*.ψ1}

{0, 0, 0}
```

UT = {ψ1, ψ2, ψ3}

$$\left\{\left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}, \{0, 0, 1\}, \left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}\right\}$$

U = Transpose[UT]

$$\left\{\left\{\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right\}, \left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \{0, 1, 0\}\right\}$$

UH = UT*

$$\left\{\left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}, \{0, 0, 1\}, \left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right\}\right\}$$

UH.U

{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

UH.A.U // Simplify

{{2, 0, 0}, {0, 0, 0}, {0, 0, 0}}

% // MatrixForm

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$