Eigenvalue and Eigenvectors of operators

The ket $|\alpha\rangle$ is called the eigenvector or eigenket of the operator A if

$$A|\alpha\rangle = \alpha|\alpha\rangle \quad \cdots\cdots\cdots (1)$$

The number α is called the eigenvalue. Thus the effect of $\hat{A}$ on an eigenket of A is merely multiplication by a number.

Eigenvalues and eigenvectors of a hermitian operator

We now take up the eigenvalue problem of hermitian operators. Two theorems are of vital importance in this context.

Theorem. The eigenvalues of a hermitian operator are real.

Theorem The ~~eigenvalues~~ eigenvectors of a hermitian operator belonging to different eigenvalues are orthogonal.

<u>Proof</u> Let A be a hermitian operator and

$$A|\alpha_1\rangle = \alpha_1 |\alpha_1\rangle \quad \cdots\cdots (1)$$

$$A|\alpha_2\rangle = \alpha_2 |\alpha_2\rangle . \quad \cdots\cdots (2)$$

From (1) we have

$$\langle\alpha_2|A|\alpha_1\rangle = \alpha_1 \langle\alpha_2|\alpha_1\rangle \quad \cdots\cdots (3).$$

Next, we take the adjoint of eq. (2).

$$\langle\alpha_2|A^\dagger = \alpha_2^* \langle\alpha_2|$$

Since A is hermitian, i.e., $A^\dagger = A$, we get

$$\langle\alpha_2|A = \alpha_2^* \langle\alpha_2|$$

Hence

$$\langle\alpha_2|A|\alpha_1\rangle = \alpha_2^* \langle\alpha_2|\alpha_1\rangle \quad \cdots\cdots (4).$$

Combining eqs. (3) and (4) we get

$$(\alpha_1 - \alpha_2^*) \langle\alpha_2|\alpha_1\rangle = 0 . \quad \cdots\cdots (5)$$

If we let $\alpha_2 = \alpha_1$, and recalling that $\langle\alpha_1|\alpha_1\rangle \neq 0$, it follows that

$$\alpha_1 - \alpha_1^* = 0$$

i.e., α_1 is real. Since eigenvalues are proved to be real, we can write Eq. (5) as

$$(\alpha_1 - \alpha_2)\langle\alpha_2|\alpha_1\rangle = 0 .$$

If $\alpha_1 \neq \alpha_2$, we must have

$$\langle\alpha_2|\alpha_1\rangle = 0$$

i.e., eigenvectors belonging to different eigenvalues are orthogonal. Owing to the linearity of the operator $\hat{A}$ we can normalize the eigenvectors. We shall therefore usually assume that

$$\langle\alpha_1|\alpha_2\rangle = \delta_{\alpha_1\alpha_2} .$$

Thus, the eigenvectors of a hermitian operator form an orthonormal (and hence linearly independent set of vectors, i.e.,

$$\langle\alpha_i|\alpha_j\rangle = \delta_{\alpha_i\alpha_j} .$$

Determination of eigenvalues and eigenvectors of a hermitian operator.

Let A be a hermitian operator. Consider the eigenvalue equation

$$A|\lambda\rangle = \lambda|\lambda\rangle . \quad \cdots\cdots (6)$$

To find the eigenvalues and the corresponding eigenvectors, we have to choose a basis in the vector space and convert the operator equation (Eq. (6)), into a matrix equation. For simplicity, we will assume that the vector space is finite dimensional with dimension n.

Now, choosing an orthonormal basis set $\{|u_i\rangle\}$, we can cast Eq. (6) as a matrix equation of the following form:

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} . \quad \cdots (7)$$

Here $x_1, x_2, \ldots, x_n$ are the components of the eigenvector $|\lambda\rangle$ in "directions" $|u_1\rangle, |u_2\rangle \cdots |u_n\rangle$, respectively, i.e.,

$$x_i \equiv \langle u_i|\lambda\rangle \; ; \quad i = 1, 2, \cdots, n \, .$$

Eq. (7) is a set of linear homogeneous equations which possess non-trivial solutions only if

$$\begin{vmatrix} (A_{11}-\lambda) & A_{12} & \cdots & A_{1n} \\ A_{21} & (A_{22}-\lambda) & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & (A_{nn}-\lambda) \end{vmatrix} = 0 , \quad \cdots (8)$$

or, in short

$$\det \left(A_{ij} - \lambda \, \delta_{ij} \right) = 0 \, .$$

In matrix notation, we can write

$$\left| \underline{A} - \lambda \, \underline{\mathbb{1}} \right| = 0 \, .$$

This equation, which is a polynomial equation of degree n in the unknown λ, is called the secular equation of the matrix (A_{ij}). Solving this equation, we get n roots which we label as

$$\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_n .$$

Now, we can distinguish two cases. If the n eigenvalues are all distinct, we say that the eigenvalues are non-degenerate. However, it may so happen that some of the eigenvalues are repeated. Those eigenvalues which are repeated are called degenerate eigenvalues and the number of times an eigenvalue is repeated is called the order of degeneracy of that eigenvalue.

Non-degenerate roots

In this case all the roots λ_i are distinct and there are n of them if the vector space is n-dimensional. If A is hermitian, the roots are real. For a non-hermitian operator some or all of the roots ~~are dist~~ may be complex.

Now, for each eigenvalue (root of secular equation) we can solve the eigenvalue equation (Eq. (7)) to get n linearly independent eigenvectors $|\lambda_i\rangle$. Since the $|\lambda_i\rangle$'s are linearly independent, they span the n-dimensional vector space, i.e., they form a complete set of basis vectors.

If A is hermitian, the eigenvectors are guaranteed to be orthogonal, i.e., $\langle \lambda_i | \lambda_j \rangle = 0$ if $i \neq j$. However, for a non-hermitian operator the eigenvectors may or may not be orthogonal.

Using the eigenvectors of A as the basis (this basis is called the eigenbasis of A), the matrix representation of A is

$$A'_{ij} \equiv \langle \lambda_i | A | \lambda_j \rangle = \lambda_j \langle \lambda_i | \lambda_j \rangle \quad \text{.....} \quad (8)$$

For hermitian A, we always have $\langle \lambda_i | \lambda_j \rangle = 0$ if $i \neq j$, and, further we can normalize each eigenvector $|\lambda_i\rangle$. Thus, for a hermitian operator, the eigenbasis is an orthonormal set, i.e.,

$$\langle \lambda_i | \lambda_j \rangle = \delta_{ij} . \quad \text{......} \quad (9)$$

Therefore, the matrix representation of the operator A in its eigenbasis ~~assumes~~ is diagonal, i.e.,

$$A'_{ij} = \lambda_j \delta_{ij} \quad \text{....} \quad (9)$$

Writing out the matrix (A'_{ij}) in full we have

$$\underline{A}' = \begin{bmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_n \end{bmatrix}.$$

An operator or a matrix $\underline{A}$ is said to be diagonalizable, if we can find a basis in which the matrix becomes diagonal. For a hermitian operator we can always find a basis, the eigenbasis of the operator, in which the matrix representation of the operator is diagonal with the eigenvalues as the diagonal elements.

For a non-hermitian operator in an n-dimensional vector space, there is no guarantee that the matrix representation A'_{ij} in the eigenbasis of the operator is diagonal. This is because, in general, the eigenvectors are not orthogonal, i.e., $\langle \lambda_i | \lambda_j \rangle \neq \delta_{ij}$.

Degenerate eigenvalues

The secular equation, (Eq. (8)), may have roots some or all of which are repeated. So, the number of distinct eigenvalues is now less than the dimension of the vector space.

As an example, suppose we have a six-dimensional vector space ($n = 6$) with three distinct roots

$$\lambda_1, \lambda_2, \lambda_3 .$$

Suppose λ_1 is repeated three times, λ_2 is repeated two times and λ_3 occurs only once. Thus the six roots of the secular equation are

$$\lambda_1, \lambda_1, \lambda_1, \lambda_2, \lambda_2, \lambda_3 .$$

We say λ_1 is three-fold degenerate, λ_2 is two-fold degenerate and λ_3 is non-degenerate. We represent the order of degeneracy of a distinct eigenvalue λ_i by g_{λ_i}. In the present example, $g_{\lambda_1} = 3$, $g_{\lambda_2} = 2$ and $g_{\lambda_3} = 1$. We have

$$g_{\lambda_1} + g_{\lambda_2} + g_{\lambda_3} = 6 \quad \text{(dimension of the vector space)}$$

Now, it may be shown that, for a <u>hermitian operator</u> if a root λ is g-fold degenerate, there are always g linearly independent eigenvectors corresponding to λ. For a non-hermitian operator, there may not exist as many linearly independent eigenvectors as the order of degeneracy.

In the above example, if λ_1, λ_2 and λ_3 are eigenvalues of a hermitian operator, there are three linearly independent eigenvectors with eigenvalue λ_1, two linearly independent eigenvectors with eigenvalue λ_2 and one eigenvector with eigenvalue λ_3. Thus, the total number of linearly independent eigenvectors is six, the same as the dimension of the vector space. Hence these six linearly independent eigenvectors form a complete basis set of vectors.

If, however, λ_1, λ_2 and λ_3 are eigenvalues of a non-hermitian operator with the same order of degeneracy for the eigenvalues, there may not exist three linearly independent eigenvectors with eigenvalue λ_1, or two linearly

independent

eigenvectors with eigenvalue λ_2. In such a situation, the number of linearly independent eigenvectors of the non-hermitian operator A is less than the dimension n of the vector space. Hence, these eigenvectors do not form a basis set for the n-dimensional vector space.

Diagonalization of a hermitian operator

Let A be a hermitian operator with distinct eigenvalues $\lambda_1, \lambda_2, \ldots$. Some or all of the eigenvalues may be degenerate, with the order or degree of degeneracy of an eigenvalue λ_i being denoted by g_{λ_i}. If $g_{\lambda_j} = 1$ for some λ_j, then λ_j is said to be non-degenerate.

Since A is hermitian there will always be g_{λ_i} linearly independent eigenvectors, each belonging to the same eigenvalue λ_i. We will now require another index, $s^{(i)}$, to distinguish between these linearly independent eigenvectors.

We write

$$A\,|\lambda_i, s^{(i)}\rangle = \lambda_i\,|\lambda_i, s^{(i)}\rangle \; ; \; s^{(i)} = 1, 2, \cdots, g_{\lambda_i} \qquad ---(9)$$

A linear combination of the degenerate eigenvectors is also an eigenvector A with the same eigenvalue λ_i. ~~Thus~~ So we have

$$A\left(\sum_{s^{(i)}=1}^{g_{\lambda_i}} C_{s^{(i)}}\,|\lambda_i, s^{(i)}\rangle\right) = \lambda_i \left(\sum_{s^{(i)}=1}^{g_{\lambda_i}} C_{s^{(i)}}\,|\lambda_i, s^{(i)}\rangle\right). \qquad ----(10)$$

Thus, the set of vectors

$$\left\{ |\lambda_i, s^{(i)}\rangle ; \ \lambda_i \text{ fixed}, \ s^{(i)} = 1, 2, \cdots g_{\lambda_i} \right\}$$

spans a subspace, called the eigen subspace of λ_i, of the original n-dimensional vector space. The eigenvectors belonging to a degenerate eigenvalue need not be orthogonal to each other even if they are linearly independent, as the general theorem of hermitian operators proves the orthogonality of eigenvectors belonging to different eigenvalues.

However, using Schmidt orthonormalization procedure, we can get a set of g_{λ_i} orthonormal eigenfunctions of eigenvalue λ_i from a set of g_{λ_i} linearly independent set of eigenfunctions of eigenvalue λ_i.

Thus, all the eigenvectors of the hermitian operator, whether ~~belo~~ belonging to same or different eigenvalues can be considered as orthogonal to each other. Further, they are also normalized.
Using the set of orthonormal eigenfunctions as the basis, ~~the matrix representation as the basis~~, the matrix representation of A is diagonal.

As a concrete example of diagonalization of a hermitian operator, suppose we have a finite seven-dimensional linear vector space. If, all the eigenvectors are ~~non-degenerate~~ non-degenerate, then there are seven distinct eigenvalues $\lambda_1, \lambda_2, \cdots \lambda_7$ and corresponding to each eigenvalue there will be one ~~d~~ eigenvector : $|\lambda_1\rangle, |\lambda_2\rangle, \cdots |\lambda_n\rangle$. These eigenvectors are orthogonal and they are normalized.
Using these eigenvectors as the basis, the matrix representation A is

$$\underline{A} = \begin{bmatrix} \lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \lambda_5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda_6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda_7 \end{bmatrix}.$$

But if some of the eigenvalues are degenerate, then the number of distinct eigenvalues will be less than seven. Suppose that there are three distinct eigenvalues

$$\lambda_1, \lambda_2, \lambda_3,$$

Also suppose that λ_1 is three-fold degenerate and λ_2 and λ_3 are both 2-fold degenerate. Thus

$$g_{\lambda_1} = 3$$

$$g_{\lambda_2} = 2$$

$$g_{\lambda_3} = 2$$

and

$$g_{\lambda_1} + g_{\lambda_2} + g_{\lambda_3} = 7 \text{ (The dimension of the vector space).}$$

There are three linearly independent (but not necessarily orthogonal) eigenvectors with eigenvalue λ_1 and two linearly independent eigenvectors for each eigenvalue λ_2 and λ_3.

The eigenvectors ~~of~~ with eigenvalue λ_1 can be labelled as

$$|\lambda_1, s^{(1)}\rangle, \quad s^{(1)} = 1, 2, 3$$

i.e

$$|\lambda_1, 1\rangle, \; |\lambda_1, 2\rangle, \; |\lambda_1, 3\rangle$$

These three eigenvectors span a subspace of the original seven-dimensional vector space H. The subspace is called the eigensubspace of λ_1 and is denoted by H_{λ_1} or simply H_1.

The eigenvectors belonging to λ_2 and λ_3 are labelled similarly. The two linearly independent eigenvectors with eigenvalue λ_2 span a two-dimensional subspace H_2 and the two linearly independent vectors belonging to λ_3 span the eigensubspace H_3. These three subspaces make up the full vector space H.

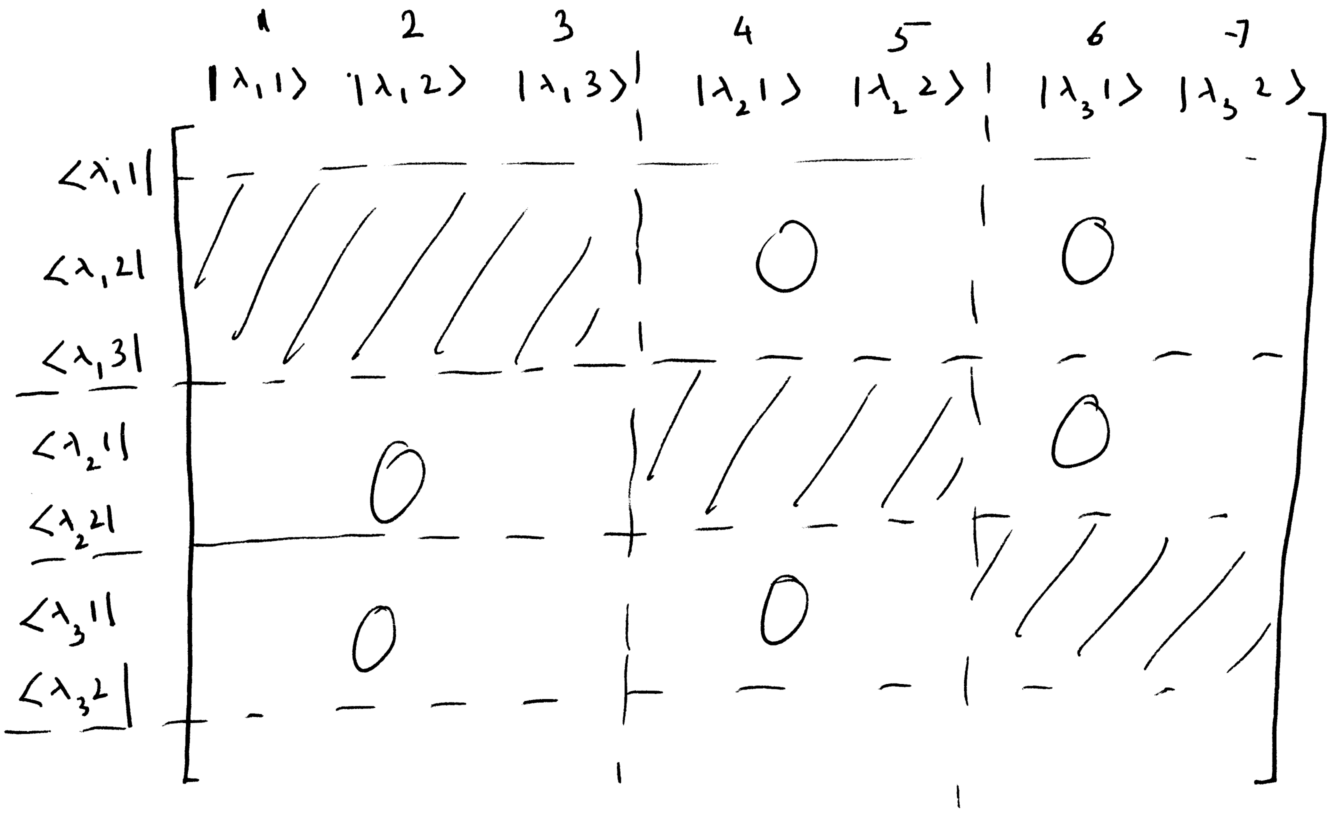
We write

$$H = H_1 \oplus H_2 \oplus H_3 .$$

The seven linearly independent eigenvectors

$$\{ |\lambda_i, s^{(i)}\rangle, s^{(i)} = 1, 2, \cdots g_{\lambda_i}, i = 1, 2, 3 \}$$

can now be used as a basis to find the matrix representation of A. If the basis vectors within an eigensubspace are not made orthogonal, the matrix representation of A is block-diagonal as shown below.



Each shaded block is a square matrix. ~~For exam~~ The first block is a 3×3 matrix, the 2nd one is a 2×2 matrix and the third one is a 2×2 matrix. These blocks themselves are not diagonal if the basis vectors of the three eigensubspaces are not orthonormalized. If we orthonormalize the basis vectors in each eigensubspace, then each ~~do~~ block will also be diagonal. The matrix representation of A will then be

$$
\begin{array}{c}
\\
\langle\lambda_1 1| \\
\langle\lambda_1 2| \\
\langle\lambda_1 3| \\
\langle\lambda_2 1| \\
\langle\lambda_2 2| \\
\langle\lambda_3 1| \\
\langle\lambda_3 2|
\end{array}
\begin{array}{c}
\begin{array}{ccccccc}
|\lambda_1 1\rangle & |\lambda_1 2\rangle & |\lambda_1 3\rangle & |\lambda_2 1\rangle & |\lambda_2 2\rangle & |\lambda_3 1\rangle & |\lambda_3 2\rangle
\end{array} \\
\left[\begin{array}{ccc|cc|cc}
\lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \lambda_1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \lambda_1 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & \lambda_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \lambda_2 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & \lambda_3 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \lambda_3
\end{array}\right]
\end{array}
$$

Thus the matrix representation of a hermitian operator A is diagonalized.

We have proved that a hermitian operator (or a hermitian matrix) is always diagonalizable in a finite dimensional vector space. By diagonalizable we mean that we can always find a basis in which the matrix representation of A is diagonal. This basis is simply the basis consisting of the orthonormalized eigenvectors of A, called the eigenbasis of A.

~~The eigenbasis of~~

The eigenvectors of a non-hermitian operator may be fewer in number than the dimension of the vector space if there is degeneracy. If an eigenvector λ_i is g_i-fold degenerate, then the number of linearly independent eigenvectors belonging to λ_i may be less than g_i. Therefore, the eigenvectors of a non-hermitian operator cannot form a basis set for the vector space. Therefore, a non-hermitian operator is not diagonalizable.

Basis independence (i.e., representation independence) of the eigenvalues of an operator.

To find the eigenvalues of a hermitian operator $\hat{A}$, first we choose an orthonormal basis set $\{|u_i\rangle\}$ and form the matrix representation of the operator. Then we solve the secular equation to find the eigenvalues. Although we have to introduce a basis set to find the eigenvalues, it is easy to verify that the eigenvalues are independent of the choice of the basis.

Indeed, if we choose a new orthonormal set of basis vectors $\{|u_i'\rangle\}$ which are related to the old set according to

$$|u_i'\rangle = \sum_j |u_j\rangle\langle u_j|u_i'\rangle$$

then the new matrix representation of the operator A is related to the old representation by a similarity transformation with a unitary matrix. This is easy to see:

$$A'_{ij} \equiv \langle u_i' | A | u_j' \rangle$$

$$= \sum_{jk} \langle u_i' | u_j \rangle \langle u_j | A | u_k \rangle \langle u_k | u_j' \rangle$$

$$= \sum_{jk} S_{ij} \, A_{jk} \, S^*_{jk}$$

$$= \sum_{jk} S_{ij} \, A_{jk} \, S^\dagger_{kj} \qquad \text{——(11)}$$

where we have defined the matrix $\underline{S}$ as

$$S_{ij} \equiv \langle u_i' | u_j \rangle .$$

The matrix $\underline{S}$ is unitary as shown previously.

In matrix notation, we write eq. (11) as

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

since $\underline{S}$ is a unitary matrix. Then

$$\det(\underline{A}' - \lambda\,\underline{I}) = \det(\underline{S}\,\underline{A}\,\underline{S}^{-1} - \lambda\,\underline{S}\,\underline{I}\,\underline{S}^{-1})$$

$$= \det(\underline{S}\,(\underline{A} - \lambda\,\underline{I})\,\underline{S}^{-1})$$

$$= \det(\underline{A} - \lambda\,\underline{I}) .$$

Thus, there is no change in the secular equation even if we change the basis set. Since the eigenvalues are the roots of the secular equation, the eigenvalues are representation independent. They are characteristics of the operator $\hat{A}$ itself, and not of any particular representation.

Next, we will show that the determinant and the trace of the matrix representation of A are independent of the basis used for the representation.

Since
$$\underline{A}' = \underline{S}\,\underline{A}\,\underline{S}^{-1}$$
we have
$$\det(\underline{A}') = \det(\underline{S}\,\underline{A}\,\underline{S}^{-1}) = \det(\underline{S}^{-1}\underline{S}\,\underline{A})$$
$$= \det(\underline{A})$$
i.e., determinant is independent of the representation.

We also have

$$\mathrm{Tr}(\underline{A}') = \mathrm{Tr}(\underline{S}\,\underline{A}\,\underline{S}^{-1}) = \mathrm{Tr}(\underline{S}^{-1}\underline{S}\,\underline{A}) = \mathrm{Tr}\,\underline{A}$$

i.e., the trace is also independent of the representation. In the above derivations, we have used the identities
$$\det(\underline{A}\,\underline{B}) = \det(\underline{B}\,\underline{A})$$
$$\mathrm{Tr}(\underline{A}\,\underline{B}) = \mathrm{Tr}(\underline{B}\,\underline{A}).$$

Now, if we use the eigenbasis of the hermitian operator A for the representation, then $\underline{A}$ is a diagonal matrix with
$$\det \underline{A} = \lambda_1 \lambda_2 \cdots \quad (\text{product of eigenvalues})$$
$$\mathrm{tr}\,\underline{A} = \lambda_1 + \lambda_2 + \cdots \quad (\text{sum of eigenvalues}).$$

If an eigenvalue is g-fold degenerate, then that eigenvalue has to be repeated g times while calculating the determinant and trace of the matrix $\underline{A}$.

Infinite dimensional vector space

We have shown that a linear operator in a finite n-dimensional vector space has n eigenvalues some of which may be repeated. If the operator is hermitian, then the eigenvalues are real and eigenvectors belonging to different eigenvalues are orthogonal and hence linearly independent.

Further, if an eigenvalue λ of a hermitian operator is g-fold degenerate, then there are g linearly independent eigenvectors corresponding to λ. These degenerate eigenvectors are not necessarily orthogonal even if they are linearly independent. However, we can orthonormalize the degenerate eigenvectors using the ~~Schmidt~~ Schmidt orthonormalization procedure.

Thus in a finite n-dimensional vector space, the eigenvectors of <u>any</u> hermitian operator form a set of orthonormal basis's ~~set~~, vectors.

In an infinite-dimensional vector space, the number of eigenvalues and eigenvectors of a hermitian operator are infinitely many. However, it is possible that the eigenvectors of some hermitian operators do not form a complete basis set in an infinite dimensional vector space.

Hermitian operators are of vital importance in quantum mechanics because to every observable like position, linear momentum, angular momentum, spin etc., we associate a corresponding hermitian operator. Of course, there are hermitian operators which are not associated with any observable.

The eigenvectors of a hermitian operator representing a physical observable form a complete set even in an infinite-dimensional Hilbert space. The eigenvectors of a hermitian operator not associated with any observable may not form a complete basis set in an infinite dimensional space.

Completeness condition for the eigenvectors of a hermitian operator

Let us assume that the eigenvalue spectrum of a hermitian operator $\hat{A}$ form a discrete set. In other words, the eigenvalues a_i, $i = 1, 2, \cdots$ of the operator are discrete real numbers.

Assume, for the time being, that the eigenvalues are non-degenerate so that there is only one linearly independent eigenvector $|a_i\rangle$ corresponding to each eigenvalue a_i. The eigenvectors $\{|a_i\rangle, i = 1, 2, \cdots\}$ form a complete orthonormal set of basis vectors. Therefore, an arbitrary vector $|\psi\rangle$ of the vector space can be expanded as a linear combination of the vectors in the basis set, i.e

$$|\psi\rangle = \sum_i c_i |a_i\rangle$$

where $c_i = \langle a_i|\psi\rangle$. Therefore, we can write

$$|\psi\rangle = \sum_i \langle a_i|\psi\rangle |a_i\rangle = \sum_i |a_i\rangle\langle a_i|\psi\rangle$$

Since $|\psi\rangle$ is arbitrary, we must have

$$\hat{\mathbb{1}} = \sum_i |a_i\rangle\langle a_i| = \sum_i \hat{P}_i \quad \cdots\cdots (1)$$

where

$$\hat{P}_i = |a_i\rangle\langle a_i| \quad \cdots\cdots\cdots (2)$$

is the projection operator along $|a_i\rangle$.

Using the basis $\{|u_i\rangle\}$, any operator $\hat{O}$ can be expressed as

$$\hat{O} = \hat{\mathbb{1}}\hat{O}\hat{\mathbb{1}} = \sum_{i,j} |a_i\rangle\langle a_i|\hat{O}|a_j\rangle\langle a_j|$$

$$= \sum_{ij} |a_i\rangle O_{ij} \langle a_j| \quad \ldots\ldots (3)$$

where $O_{ij} \equiv \langle a_i|\hat{O}|a_j\rangle$ are the matrix elements of $\hat{O}$ in the basis $\{|u_i\rangle\}$. Since the basis is the eigenbasis of the operator $\hat{A}$, the matrix elements of $\hat{A}$ in the basis will be diagonal, i.e.,

$$A_{ij} = \langle a_i|\hat{A}|a_j\rangle = a_i\delta_{ij}$$

so that we can write

$$\hat{A} = \sum_i a_i|a_i\rangle\langle a_i| = \sum_i a_i \hat{P}_i \quad \ldots\ldots (4)$$

Any other operator $\hat{B}$ will in general not be diagonal in the eigenbasis of $\hat{A}$ unless the eigenvectors of $\hat{B}$ and $\hat{A}$ coincide. Later, we will see that two operators $\hat{A}$ and $\hat{B}$ have simultaneous eigenvectors if they commute, i.e., if $[\hat{A}, \hat{B}] = 0$.

Now, we will generalize the notation to include degeneracy. Suppose the eigenvalue a_i is g_i-fold degenerate. Then the eigenvectors belonging to the eigenvalue a_i is written as

$$|a_i, s^{(i)}\rangle$$

where $s^{(i)}$ can take values $1, 2, \cdots g_i$. The set of vectors

$$\left\{ |a_i, s^{(i)}\rangle, \; s^{(i)} = 1, 2, \cdots g_i \; ; \; i = 1, 2, 3, \cdots \right\}$$

form a complete orthonormal set. The completeness condition is

$$\sum_{i=1}^{\infty} \sum_{s^{(i)}=1}^{g_i} |a_i, s^{(i)}\rangle\langle a_i, s^{(i)}| = \hat{\mathbb{1}} \quad \cdots (5)$$

and the orthonormality condition is

$$\langle a_i, s^{(i)} | a_j, s^{(j)} \rangle = \delta_{ij}\, \delta_{s^{(i)} s^{(j)}} . \qquad \text{---} (6)$$

We can rewrite Eq. (5) as (exactly as in the nondegenerate case)

$$\hat{\mathbb{1}} = \sum_i \hat{P}_i \qquad \text{------} (7)$$

where

$$\hat{P}_i = \sum_{s^{(i)}=1}^{g_i} |a_i, s^{(i)}\rangle\langle a_i s^{(i)}| \qquad \text{----} (8)$$

is the projection operator on the eigensubspace of a_i. The operator $\hat{A}$ can then be written in its own eigenbasis as

$$\hat{A} = \sum_i a_i \hat{P}_i$$

with $\hat{P}_i$ given in (8).

Hermitian operators with continuous eigenvalue spectrum.

In Quantum Mechanics we encounter hermitian operators like position operator, momentum operator whose eigenvalues range over a continuum of real values. Such an eigenvalue spectrum is called continuous. There are also hermitian operators whose eigenvalue spectrum may be both discrete and continuous.

Continuous spectrum.

Let us consider an operator A whose eigenvalues can vary continuously over a certain ~~range~~ domain of real numbers.

$$A|a\rangle = a|a\rangle \quad - - - - - (9)$$

If there is degeneracy, we will put in a second index s to distinguish between the degenerate vectors. Thus we may write $|a\, s\rangle$ to denote a degenerate eigenvector. We assume that there is no degeneracy. In case of degeneracy it is a simple matter to generalize our notations. We assume that the vectors $|a\rangle$ form a complete set. The completeness condition can be written as

$$\int da\, |a\rangle\langle a| = \hat{\mathbb{1}} \quad - - - - - (10)$$

where the integral extends over the entire domain in which a varies. Usually this domain is $-\infty$ to ∞.

Two eigenkets $|a\rangle$ and $|a'\rangle$ with $a \neq a'$ are orthogonal because A is a hermitian operator, i.e.,

$$\langle a|a'\rangle = 0 \,;\; a \neq a'. \quad - - - (11)$$

What will the scalar product be if $a = a'$? Can we take $\langle a|a\rangle = 1$ as in the discrete case where we normalised the eigenkets as $\langle a_i|a_i\rangle = 1$?

The answer is no, i.e., in the case where the eigenvalues a vary continuously, the kets $|a\rangle$ cannot be normalized to unity. To see this, expand an arbitrary ket $|f\rangle$ in the eigenbasis $\{|a\rangle\}$ of the operator $\hat{A}$. We have

$$|f\rangle = \int da' \, |a'\rangle\langle a'|f\rangle. \quad \cdots\cdots (10)$$

Taking the scalar product of $|f\rangle$ with $|a\rangle$, we get

$$\langle a|f\rangle = \int da' \, \langle a|a'\rangle\langle a'|f\rangle$$

or,
$$f(a) = \int da' \langle a|a'\rangle f(a') \quad \cdots\cdots (11)$$

where we have defined $f(a)$ as $f(a) = \langle a|f\rangle$. In order for Eq. (11) to be valid, we must have

$$\langle a|a'\rangle = \delta(a-a'), \quad \cdots\cdots (12)$$

for, with this choice, the right side of Eq. (11) becomes equal to the left side:

$$\begin{aligned} \text{RHS of Eq. (11)} &= \int da' \, \delta(a-a') f(a') \\ &= f(a) \\ &= \text{LHS of Eq. (11)}. \end{aligned}$$

Thus, setting $a' = a$ in Eq. (12) we find

$$\langle a|a\rangle = \delta(0) = \infty .$$

In other words, the eigenkets $\{|a\rangle\}$ are not normalizable to unity since $\langle a|a\rangle$ is not finite. Therefore, the eigenkets $\{|a\rangle\}$ do not belong to the Hilbert space. However, we can ~~incl~~ include such eigenkets in the vector space, and the augmented vector space is called the <u>physical Hilbert space</u>.

The kets $\{|a\rangle\}$ are not physically realizable in the sense that no physical state of a system can have a state vector $|\psi\rangle$ which is one of the eigenkets $|a\rangle$. However, the set of eigenkets $\{|a\rangle\}$ can form a basis set because an arbitry ket $|\psi\rangle$ of finite norm can always be expanded in terms of $\{|a\rangle\}$.

As a matter of terminology, we say that the eigenkets belonging to continuously varying eigenvalues of a hermitian operator are "normalizable" to a delta function, i.e., $\langle a|a'\rangle = \delta(a-a')$, even though the kets $|a\rangle$ are not normalizable in the strict mathematical sense, since

$$\| \, |a\rangle \, \| = \infty \quad \text{(not finite)} .$$

In summary, for continuously varying eigenvalues, the orthogonality and completeness of the eigenvectors of a hermitian operator are written as

$$\langle a|a'\rangle = \delta(a-a') \quad \text{(orthogonality)}$$

$$\hat{\mathbb{1}} = \int da \, |a\rangle\langle a| \quad \text{(completeness)} .$$

Hermitian operators with both discrete and continuous eigenvalues

The eigenvalue spectrum of a hermitian operator can be both discrete and continuous. In such a situation we have

$$\hat{A}\,|a_i\rangle = a_i\,|a_i\rangle \; ; \quad i = 1, 2, \dots$$

for discrete eigenvalues, and

$$\hat{A}\,|a\rangle = a\,|a\rangle \; ; \quad a \in D \subset \mathbb{R}$$

for continuous eigenvalues. The completeness condition is

$$\sum_i |a_i\rangle\langle a_i| + \int da\, |a\rangle\langle a| = \hat{\mathbb{1}}$$

and the orthonormality conditions are:

$$\langle a_i|a_j\rangle = \delta_{ij}$$

$$\langle a|a'\rangle = \delta(a-a')$$

$$\langle a_i|a\rangle = 0 .$$

Ex Find the eigenvalues and eigenvectors of the matrix

$$M = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

Can this matrix be diagonalized?

Ans The eigenvalue eq. is

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}.$$

The secular eq. is then

$$\det(M - \lambda \underline{I}) = 0$$

or
$$\begin{vmatrix} 1-\lambda & 1 \\ 0 & 1-\lambda \end{vmatrix} = 0$$

or $(\lambda - 1)^2 = 0.$

i.e., $\lambda = 1, 1$ (2 fold degeneracy)

Eigenvector

With $\lambda = 1$, the eigenvalue eq. is

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 1 \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

or
$$\begin{pmatrix} x_1 + x_2 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

Thus

$$x_1 + x_2 = x_1$$

or

$$x_2 = 0$$

The element x_1 is arbitrary. Hence

$$|1\rangle = \begin{pmatrix} x_1 \\ 0 \end{pmatrix} \quad (x_1 \text{ arbitrary}).$$

Normalizing

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

We have found just one linearly independent eigenvector with $\lambda = 1$. Since M is not hermitian, there is no guarantee that there would be two linearly independent eigenvectors for a two-fold degenerate eigenvalue. Here, for the given matrix M, which is non-hermitian, we have only one linearly independent eigenvector corresponding to the two-fold degenerate eigenvalue $\lambda = 1$.

So we do not have a complete set of eigenvectors of M ~~whi~~ to span the two-dimensional vector space. Hence M is not diagonalizable by a change of basis, i.e., by a similarity transformation.

Ex Find the eigenvalues and the corresponding eigenvectors of the matrix

$$A = \begin{pmatrix} 3 & i \\ -i & 3 \end{pmatrix}.$$

Ans First note that $A^{+} = A$, i.e., the matrix is hermitian. Hence the eigenvalues would be real and the eigenvectors belonging to distinct eigenvalues would be orthogonal.

The eigenvalue eq. is

$$\begin{pmatrix} 3 & i \\ -i & 3 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

or $$\begin{pmatrix} 3-\lambda & i \\ -i & 3-\lambda \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \cdots \quad (1)$$

The secular equation is

$$\begin{vmatrix} 3-\lambda & i \\ -i & 3-\lambda \end{vmatrix} = 0$$

or,

$$(3-\lambda)^2 - (i)(-i) = 0$$

or $$(\lambda-3)^2 - 1 = 0$$

or $$(\lambda-3-1)(\lambda-3+1) = 0$$

or $$(\lambda-4)(\lambda-2) = 0$$

or $\lambda = 2, 4.$ (None of the roots are degenerate).

Take $\lambda_1 = 2$, $\lambda_2 = 4$.

<u>Eigenvector for $\lambda_1 = 2$</u>

Substitute $\lambda_1 = 2$ in eq. (1).

$$\begin{pmatrix} 3-2 & i \\ -i & 3-2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \phi$$ ← ϕ means $\begin{pmatrix} 0 \\ 0 \end{pmatrix}$ null matrix.

$$\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \phi$$

$$\begin{pmatrix} x_1 + i x_2 \\ -i x_1 + x_2 \end{pmatrix} = \phi$$

Thus
$$x_1 + i x_2 = 0 \quad \text{———} (2)$$
$$-i x_1 + x_2 = 0 \quad \text{———} (3)$$

From (1)

$$x_1 = -i x_2$$

Substituting in (2)

$$-i(-i x_2) + x_2 = 0$$

or $\quad -x_2 + x_2 = 0 \quad$ identity.

Take x_2 to be arbitrary.

Hence

$$|2\rangle \doteq \begin{pmatrix} -i x_2 \\ x_2 \end{pmatrix}$$

Normalizing

$$\langle 2|2\rangle = 1$$

or $\quad \begin{pmatrix} i x_2^* & x_2^* \end{pmatrix} \begin{pmatrix} -i x_2 \\ x_2 \end{pmatrix} = 1$

or $\quad 2|x_2|^2 = 1$

or $\quad |x_2| = \frac{1}{\sqrt{2}}$

Take $\quad x_2 = \frac{1}{\sqrt{2}}$.

We Could have taken

$$x_2 = -\frac{1}{\sqrt{2}}$$

or,

$$x_2 = e^{i\phi}\frac{1}{\sqrt{2}} \quad (\phi = \text{real}).$$

In all cases $|x_2| = \frac{1}{\sqrt{2}}$

$\therefore$ Normalized eigenvector $|2\rangle$ is

$$\boxed{|2\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \end{pmatrix}} \quad \text{--- (L1)}$$

Eigenvector for $\lambda_2 = 4$

Substitute $\lambda_2 = 4$ in Eq. (1).

$$\begin{pmatrix} 3-4 & i \\ -i & 3-4 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$$

or

$$\begin{pmatrix} -1 & i \\ -i & -1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$$

or

$$\begin{pmatrix} -x_1 + ix_2 \\ -ix_1 - x_2 \end{pmatrix} = 0$$

or

$$-x_1 + i x_2 = 0 \quad \text{———} \quad (5)$$

$$-i x_1 - x_2 = 0 \quad \text{———} \quad (6)$$

From (5)

$$x_1 = i x_2$$

Substitute in (6)

$$-i\,(i x_2) - x_2 = 0$$

or $\quad x_2 - x_2 = 0 \quad$ (identity)

Take x_2 as arbitrary. Thus

$$|4\rangle \doteq \begin{pmatrix} i x_2 \\ x_2 \end{pmatrix}$$

The value of x_2 has to be found from normalization:

$$\langle 4|4\rangle = 1$$

or $\quad \left(-i x_2^* \;\; x_2^*\right)\begin{pmatrix} i x_2 \\ x_2 \end{pmatrix} = 1$

or $\quad |x_2|^2 + |x_2|^2 = 1$

or $\quad |x_2| = \frac{1}{\sqrt{2}}$

Take

$$x_2 = \frac{1}{\sqrt{2}} .$$

Hence

$$\boxed{|4\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix}} \quad \cdots\cdots \quad (7)$$

<u>Orthogonality of the eigenvectors.</u>

$$|2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \end{pmatrix}$$

$$|4\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix}$$

$$\langle 2|4\rangle = \frac{1}{2}\begin{pmatrix} i & 1 \end{pmatrix}\begin{pmatrix} i \\ 1 \end{pmatrix} = \frac{1}{2}\left(i^2+1\right) = \frac{1}{2}(-1+1) = 0.$$

If we take $|2\rangle$ and $|4\rangle$ as the basis, matrix representation of $\hat{A}$ is

$$\hat{A} \rightarrow \begin{pmatrix} \langle 2|\hat{A}|2\rangle & \langle 2|\hat{A}|4\rangle \\ \langle 4|\hat{A}|2\rangle & \langle 4|\hat{A}|4\rangle \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix}.$$

Now we find the similarity transformation that diagonalizes the matrix $\underline{A}$

$$\underline{A}' = \begin{array}{c} \langle 2| \\ \langle 4| \end{array} \begin{pmatrix} i/\sqrt{2} & 1/\sqrt{2} \\ -i/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \underline{A} \begin{array}{c} \begin{array}{cc} |2\rangle & |4\rangle \\ \downarrow & \downarrow \end{array} \\ \begin{pmatrix} -i/\sqrt{2} & i/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \end{array}$$

$$\underline{A}' = \begin{array}{c} \langle 2| \\ \langle 4| \end{array} \begin{pmatrix} i/\sqrt{2} & 1/\sqrt{2} \\ -i/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 3 & i \\ -i & 3 \end{pmatrix} \begin{array}{c} \begin{array}{cc} |2\rangle & |4\rangle \end{array} \\ \begin{pmatrix} -i/\sqrt{2} & i/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \end{array}$$

$$= \underline{S}\,\underline{A}\,\underline{S}^{-1}$$

<u>Ex</u> Find the eigenvalues and normalized eigenvectors of the matrix

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

<u>Ans</u>: The matrix M is hermitian. Therefore the eigenvalues are real. The eigenvalues are obtained by solving the secular equation

$$\begin{vmatrix} \frac{3}{2}-\lambda & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{3}{2}-\lambda & 0 \\ 0 & 0 & 1-\lambda \end{vmatrix} = 0$$

or $\quad (1-\lambda)\left\{\left(\frac{3}{2}-\lambda\right)^2 - \left(-\frac{1}{2}\right)\left(-\frac{1}{2}\right)\right\} = 0$

or $\quad (\lambda-1)\left\{(\lambda-3/2)^2 - \frac{1}{4}\right\} = 0$

or $\quad (\lambda-1)\left\{(\lambda-3/2+1/2)(\lambda-3/2-1/2)\right\} = 0$

or $\quad (\lambda-1)(\lambda-1)(\lambda-2) = 0$

Thus the eigenvalues are

$$\lambda = 1, 1, 2$$

The eigenvalue 1 is two-fold degenerate and the eigenvalue 2 is non-degenerate. The two distinct eigenvalues are $\lambda_1 = 1$ with $g_1 = 2$ and $\lambda_2 = 2$ with $g_2 = 1$.

<u>Consider $\lambda = 1$</u>

Since M is hermitian, there will be two linearly independent eigenvectors corresponding to $\lambda = 1$. We will make the two linearly independent eigenvectors orthonormal.

The eigenvalue equation is

$$\underline{M} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 1 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

N

$$\begin{pmatrix} \frac{3}{2} - 1 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{3}{2} - 1 & 0 \\ 0 & 0 & 1 - 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\parallel$$

$$\alpha \quad \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$N \quad \cancel{\begin{pmatrix} \frac{1}{2}x_1 - \frac{1}{2}x_2 \\ -\frac{1}{2}x_1 + \frac{1}{2}x_2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}}$$

$$N \quad \begin{pmatrix} \frac{1}{2}x_1 - \frac{1}{2}x_2 \\ -\frac{1}{2}x_1 + \frac{1}{2}x_2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Thus $x_1 = x_2 = x$ (say) with x arbitrary.

~~and~~ Also, x_3 is arbitrary.

Hence $|1\rangle$ is of the form

$$|1\rangle = \begin{pmatrix} x \\ x \\ z \end{pmatrix}$$

Choose $x = 1$ and $z = 0$, so that

$$|1\rangle^{(1)} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

Normalizing

$$\boxed{|1\rangle^{(1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \doteq |\lambda = 1, s = 1\rangle}$$

(s is the degeneracy index).

Next choose $x = 0$, $z = 1$

$$\boxed{|1\rangle^{(2)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \doteq |\lambda = 1, s = 2\rangle}$$

These are the two orthonormal eigenvectors with eigenvalue $\lambda = 1$.

Next, consider $\lambda = 2$

$\lambda = 2$, degeneracy $g_{\lambda=2} = 1$. The eigenvalue eq. is

$$\begin{pmatrix} \frac{3}{2}-2 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{3}{2}-2 & 0 \\ 0 & 0 & 1-2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

or

$$\begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

or

$$\begin{pmatrix} -\frac{1}{2}x_1 - \frac{1}{2}x_2 \\ -\frac{1}{2}x_1 - \frac{1}{2}x_2 \\ -x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

So we must have

$x_1 = -x_2 = x$ (say) x is arbitrary.

$x_3 = 0$.

Therefore, eigenvector $|2\rangle$ is of the form

$$|2\rangle = \begin{pmatrix} x \\ -x \\ 0 \end{pmatrix}$$

Normalizing

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

Similarity transformation.

$$\underline{M}' = \underline{S}\,\underline{M}\,\underline{S}^{\dagger}$$

Now

$$\begin{array}{cccc} & |11\rangle & |12\rangle & |2\rangle \\ & \downarrow & \downarrow & \downarrow \\ \underline{S}^{\dagger} = & \multicolumn{3}{c}{\begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{bmatrix}} \end{array}$$

$$\therefore \underline{S} = \left(S^{+}\right)^{+} = \begin{array}{l} \langle 1,1| \rightarrow \\ \langle 1,2| \rightarrow \\ \langle 2| \rightarrow \end{array} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

The matrix M' is diagonal.

$$\underline{M}' = \underline{S}\,\underline{M}\,\underline{S}^{+} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$