The eigenvalues of a unitary operator lie on the unit circle in \( \mathbb{C} \), i.e. are complex numbers with unit modulus. Their eigenvectors are mutually orthogonal (for degenerate situations, this will be achieved in the same way as for Hermitian operators).

Proof (assuming no degeneracy for simplicity)

\[ \hat{U} |u_i\rangle = u_i |u_i\rangle, \hat{U} |u_j\rangle = u_j |u_j\rangle \]

\[ \langle u_j | U^* U | u_i \rangle = u_j u_j^* \langle u_j | u_i \rangle = \hat{I} \]

\[ \Rightarrow (1 - u_i u_i^*) \langle u_j | u_i \rangle = 0 \]

For \( i = j \):

\( 1 - u_i u_i^* = 0 \) since \( \langle u_i | u_i \rangle \neq 0 \) \( \Rightarrow |u_i|^2 = 1 \)

For \( i \neq j \):

Since \( |u_i\rangle \neq |u_j\rangle \) \( \Rightarrow u_i + u_j \Rightarrow u_i u_i^* + u_j u_j^* = 1 \)

hence \( u_i u_i^* + 1 \) and therefore \( \langle u_j | u_i \rangle = 0 \) \( \square \)

Diagonalization of Hermitian or unitary matrices:

Consider an orthonormal basis

\[ |1\rangle, |2\rangle, \ldots, |n\rangle \] in \( \mathbb{V}^n(\mathbb{C}) \)

The orthonormalized eigenstates \( |w_1\rangle, \ldots, |w_n\rangle \) of a Hermitian or unitary operator \( \hat{\Omega} \) can be expanded in this basis as

\[ |w_i\rangle = \sum_k u_{ik} |k\rangle \]

where \( u_{ik} \) is the \( k \)th component of \( |w_i\rangle \) in the basis \( \{ |k\rangle \}, k = 1, \ldots, n \).
In the basis $|w_i\rangle$ the operator is diagonal:

$$\langle w_i | \hat{\mathbf{S}} | w_j \rangle = w_i \delta_{ij} \quad \rightarrow \quad (w_1, w_2, \ldots, w_n)$$

$$C = \sum_{k'} \langle k' | u^*_{kk'} | \hat{\mathbf{S}} | \sum_{k} u_{jk} | k \rangle$$

$$= \sum_{kk'} u^*_{kk'} \delta_{kk'} u_{jk} = (U^T + \hat{\mathbf{S}} U)_{ij}$$

$U^T$ is a unitary matrix made up from the orthonormal eigenvectors $|w_i\rangle$ in the basis $\{|k\rangle\}$. We see that $\hat{\mathbf{S}}$ is diagonalized by a unitary transformation with the unitary matrix $U$.

$\Rightarrow$ Any Hermitian matrix can be diagonalized by a unitary matrix $U$ (built from the eigenvectors of $\hat{\mathbf{S}}$) by forming $U^T \hat{\mathbf{S}} U$.

$\Rightarrow \text{Corollary: The determinant of a Hermitian or unitary operator is given by the product of its eigenvalues.}$

**Proof:**

$$\det (\hat{\mathbf{S}}) = \det (U^T \hat{\mathbf{S}} U) = \det (U^T) \det (\hat{\mathbf{S}}) \det (U)$$

$$= \det (\hat{\mathbf{S}}) \det (U^T U)$$

Take for $\hat{\mathbf{S}}$ the operator that diagonalizes $\hat{\mathbf{S}}$ and you are done.
Simultaneous diagonalization of two Hermitian operators

Theorem: If $\hat{\Sigma}$ and $\hat{\Lambda}$ are two commuting Hermitian operators, $[\hat{\Sigma}, \hat{\Lambda}] = 0$, then there exists (at least) a basis of common eigenvectors that diagonalizes both.

Proof: Consider first the case that at least one of the two operators, say $\hat{\Sigma}$, is nondegenerate (i.e., each eigenvalue has only one normalized eigenvector):

$$\hat{\Sigma}|w_i\rangle = \omega_i|w_i\rangle \Rightarrow \hat{\Lambda}\hat{\Sigma}|w_i\rangle = \omega_i \hat{\Lambda}|w_i\rangle$$

Since $[\hat{\Lambda}, \hat{\Sigma}] = 0$ then

$$\hat{\Sigma}(\hat{\Lambda}|w_i\rangle) = \omega_i (\hat{\Lambda}|w_i\rangle)$$

$\hat{\Lambda}|w_i\rangle$ is also an eigenvector of $\hat{\Sigma}$, with the same eigenvalue. Since the eigenvectors of $\hat{\Lambda}$ were assumed to be unique, up to a scale $\Rightarrow \hat{\Lambda}|w_i\rangle = \omega_i|w_i\rangle$.

Now the more complex case where both operators have degenerate eigenvalues. Let us reorder the eigenstates such that in its eigenbasis $\hat{\Sigma}$ is represented by the diagonal matrix

$$\hat{\Sigma} \leftrightarrow \begin{pmatrix} \omega_1 & & & \\ & \ddots & & \\ & & \omega_k & \\ & & & \omega_{\ell} \end{pmatrix}$$

Note that this eigenbasis is not unique. In the subspace $V_{w_i} = V_{w_i}$ corresponding to eigenvalue $\omega_i$, there exist an infinity of bases, let us pick one such set and label the eigenstate as $|w_i, \alpha\rangle$ where $\alpha = 1, 2, \ldots, m_i$. In this basis, what are the matrix elements of $\hat{\Lambda}$?

Look at

$$<\hat{\Sigma}\hat{\Lambda}|w_i, \alpha\rangle = \Lambda_{\alpha\beta} <\hat{\Sigma}|w_i, \beta\rangle = \omega_i \Lambda_{\alpha\beta} <\hat{\Lambda}|w_i, \beta\rangle$$
So $|w_i, \alpha \rangle$ is an eigenstate of $\hat{\Sigma}$ with eigenvalue $w_i$, i.e., it lies in $V_i^m$ but can be an arbitrary superposition of the basis states $|w_i, \alpha \rangle |\alpha = 1, 2, \ldots, m_i \rangle$. On the other hand, since eigenstates from different eigenvalues are orthogonal, $\langle w_j, \beta | w_i, \alpha \rangle = 0$ for $i \neq j$, for any $\alpha, \beta$, we can conclude that $\langle w_j, \beta | \hat{\Lambda} | w_i, \alpha \rangle = 0$. Hence, in the chosen basis, $\hat{\Lambda}$ is represented by the block-diagonal matrix

\[
\hat{\Lambda} = \begin{pmatrix}
\Lambda_1 & \vdots & \Lambda_k \\
\vdots & \ddots & \vdots \\
\Lambda_{m_1} & \cdots & \Lambda_{m_k}
\end{pmatrix}
\]

Now consider one of the block matrices $\Lambda_i$, acting on vectors in $V_i^m$. As $\Lambda_i$ acts on some $\hat{\Sigma}$-eigenstate $|w_i, \alpha \rangle$, it turns it into some other vector in $V_i^m$. $\Lambda_i$ is Hermitian, since $\hat{\Lambda}$ is. So we can diagonalize it by finding the basis $\{ |w_i, \alpha \rangle |\alpha = 1, 2, \ldots, m_i \}$ for an eigenbasis of $\Lambda_i$. Since the vectors of the eigenbasis are linear superpositions of the $\{ |w_i, \alpha \rangle |\alpha = 1, 2, \ldots, m_i \}$, all of which are $\hat{\Sigma}$-eigenstates with eigenvalue $w_i$, the $\Lambda_i$-eigenstates remain eigenstates of $\hat{\Sigma}$ with eigenvalue $w_i$. In the eigenbasis of $\hat{\Lambda}$, made from the eigenbasis set of $\Lambda_i$, $\hat{\Sigma}$ and $\hat{\Lambda}$ are now both represented by diagonal
If inside $\mathcal{W}_i$, $\hat{\Lambda}$ is non-degenerate, then this eigenbasis is unique. The eigenstates are the uniquely labelled by the eigenvalue $w$ of $\hat{S}_z$ and $\lambda$ of $\hat{\Lambda}$: $|w, \lambda\rangle$. If $\hat{\Lambda}_i$ is still degenerate, then we need one or more additional labels $|w, \lambda, \gamma, \ldots\rangle$, corresponding to eigenvalues of additional operators $\hat{\Pi}_i, \ldots$, that commute with both $\hat{S}_z$ and $\hat{\Lambda}$. We will henceforth assume that a complete set of commuting operators, whose eigenvalue identifies the basis vectors uniquely, always exists, even if $n$ is infinite. (For finite $n$, this is always true.)
Example from classical mechanics:

Two masses coupled to each other and two walls by springs:

\[ x_1, x_2 \] measure the displacement of the masses from their equilibrium points.

All springs have the same spring constant \( k \).

Equations of motion:

\[
\begin{align*}
\ddot{x}_1 &= -\frac{2k}{m} x_1 + \frac{k}{m} x_2 \\
\ddot{x}_2 &= +\frac{k}{m} x_1 - \frac{2k}{m} x_2
\end{align*}
\] (1) (2)

Find \( x_1(t), x_2(t) \), given initial positions and velocities.

Assume zero initial velocities for simplicity, so initial conditions are \( x_1(0), x_2(0) \).

Reformulate in language of linear vector spaces:

\[
\begin{pmatrix}
\dot{x}_1 \\
\dot{x}_2
\end{pmatrix}
= \begin{pmatrix}
\Omega_{11} & \Omega_{12} \\
\Omega_{21} & \Omega_{22}
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix}
\text{ or } \begin{pmatrix}
\ddot{x}_1 \\
\ddot{x}_2
\end{pmatrix}
= \hat{\Omega} \begin{pmatrix}
x_1 \\
x_2
\end{pmatrix}
\] (5)

\[
\Omega_{11} = \Omega_{22} = -\frac{2k}{m} \quad \Omega_{12} = \Omega_{21} = \frac{k}{m}
\]

\( \mathbf{\Omega} \in \mathbb{R}^{2\times2} \) (2 real components) \( \rightarrow \) 2-dimensional basis

\( \hat{\Omega} \) is Hermitian.

Let's introduce the following basis:

\[
\begin{align*}
|1\rangle & \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \leftrightarrow \begin{bmatrix} \text{first mass displaced by one length unit} \\
\text{second mass undisplaced} \end{bmatrix} \\
|2\rangle & \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} \leftrightarrow \begin{bmatrix} \text{first mass undisplaced} \\
\text{second mass displaced by unity} \end{bmatrix}
\end{align*}
\]
Let us project \((x)\) onto \(|1\rangle\):

\[
\langle 1 | \hat{S} | x(t) \rangle \leftrightarrow (1, 0) \begin{pmatrix} \frac{-2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = (1, 0) \begin{pmatrix} -\frac{2k}{m} x_1 + \frac{k}{m} x_2 \\ + \frac{k}{m} x_1 - \frac{2k}{m} x_2 \end{pmatrix} \]

\[\Rightarrow x_1 = -\frac{2k}{m} x_1 + \frac{k}{m} x_2 \quad \text{first E.O.M. (1)}\]

Similarly, the second E.O.M. is obtained by projecting \((x)\) onto \(|2\rangle\).

An arbitrary state of the system is given by

\[
\begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} x_1(t) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} x_2(t)
\]

or

\[|x(t)\rangle = x_1(t) |1\rangle + x_2(t) |2\rangle\]

In this basis, the matrix \(\begin{pmatrix} -\frac{2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} \end{pmatrix}\) represents the operator \(\hat{S}\) in \((x)\).

The basis \(|1\rangle, |2\rangle\) is desirable for giving the final solution in an explicit form. However, solution of the initial value problem is not easy in this basis, since \(\hat{S}\) is non-diagonal. The solution is obtained much more easily in a basis of eigenstates of \(\hat{S}\).

There will be two eigenvectors; let us call them \(|I\rangle\) and \(|II\rangle\):

\[\hat{S} |I\rangle = -\omega_{I}^{2} |I\rangle \quad \text{and} \quad \hat{S} |II\rangle = -\omega_{II}^{2} |II\rangle\]

(We call the eigenvalues \(-\omega_{I,II}^{2}\) because we know from kindergarten that this will be convenient; at this point, nothing tells us that \(\omega_{I,II}\) will not be imaginary.)
We only know from hermiticity of $J_z$ that $\omega_z^2$, $\omega_{\Pi}^2$ are real, but not that they are positive.

Let's solve the eigenvalue problem to find the eigenvalues:

The characteristic equation $\det(J^2 + \omega^2 I) = 0$

becomes

$$\begin{vmatrix}
-\frac{2k}{m} + \omega^2 & k/m \\
k/m & -\frac{2k}{m} + \omega^2
\end{vmatrix} = 0 \implies \left(\frac{-2k}{m} + \omega^2\right)^2 - \frac{k^2}{m^2} = 0$$

$$\implies \omega^2 - \frac{2k}{m} = \pm \frac{k}{m}$$

$$\implies \omega_z^2 = \frac{k}{m}, \quad \omega_{\Pi}^2 = \frac{3k}{m}$$

So the eigenfrequencies are $\omega_z = \sqrt{\frac{k}{m}}$, $\omega_{\Pi} = \sqrt{3} \omega_z$.

The corresponding eigenvectors are:

$\omega_z$:

$$\begin{pmatrix}
-\omega_z^2 & \omega_z^2 \\
\omega_z^2 & -2\omega_z^2
\end{pmatrix}\begin{pmatrix}a_1 \\ a_2\end{pmatrix} = -\omega_z^2 \begin{pmatrix}a_1 \\ a_2\end{pmatrix}$$

$$\implies -2\omega_z^2 a_1 + \omega_z^2 a_2 = -\omega_z^2 a_1 \implies a_2 = a_1$$

$$\omega_z^2 a_1 - 2\omega_z^2 a_2 = -\omega_z^2 a_2 \implies a_1 = a_2 (\text{redundant})$$

$$\implies \begin{pmatrix}1 \\ \sqrt{2}\end{pmatrix} \quad \text{(normalized)}$$

$\omega_{\Pi}$:

$$\begin{pmatrix}
-\frac{2}{3} \omega_{\Pi}^2 & \frac{1}{3} \omega_{\Pi}^2 \\
\frac{1}{3} \omega_{\Pi}^2 & -\frac{2}{3} \omega_{\Pi}^2
\end{pmatrix}\begin{pmatrix}a_1 \\ a_2\end{pmatrix} = -\omega_{\Pi}^2 \begin{pmatrix}a_1 \\ a_2\end{pmatrix}$$

$$\implies -\frac{2}{3} a_1 + \frac{1}{3} a_2 = -a_1 \quad \frac{1}{3} a_1 - \frac{2}{3} a_2 = -a_2$$

$$\implies a_2 = -\frac{1}{3} a_1 \implies a_1 = -a_2$$

$$\implies \begin{pmatrix}1 \\ -\sqrt{2}\end{pmatrix} \quad \text{redundant}$$

$$\implies \begin{pmatrix}1 \\ \sqrt{2}\end{pmatrix} \quad \text{normalized}$$
Expanding now the system's state vector in this new basis as

\[ |\bar{X}(t)\rangle = x_1(t) |I\rangle + x_\Pi(t) |\Pi\rangle \]

the components \(x_1\) and \(x_\Pi\) will evolve as follows:

\[
|10\rangle = \left(\frac{d^2}{dt^2} - \omega_1^2\right) |\bar{X}(t)\rangle = \left(\frac{d^2}{dt^2} - \omega_1^2\right) \left[ x_1(t) |I\rangle + x_\Pi(t) |\Pi\rangle \right] \\
= (\ddot{x}_1 - \omega_1^2 x_1) |I\rangle + (\ddot{x}_\Pi - \omega_\Pi^2 x_\Pi) |\Pi\rangle \\
= (\ddot{x}_1 + \omega_1^2 x_1) |I\rangle + (\ddot{x}_\Pi + \omega_\Pi^2 x_\Pi) |\Pi\rangle
\]

Projecting with \(\langle I |\) gives

\[ \dot{x}_1 = -\omega_1^2 x_1 \]

and with \(\langle \Pi |\) gives

\[ \dot{x}_\Pi = -\omega_\Pi^2 x_\Pi \]

These equations are decoupled and easily solved. With vanishing initial velocities the solutions are

\[ \begin{align*}
 x_1(t) &= x_1(0) \cos(\omega_1 t) \\
 x_\Pi(t) &= x_\Pi(0) \cos(\omega_\Pi t)
\end{align*} \]

\[
|\bar{X}(t)\rangle = \frac{x_1(t)}{\langle I |\bar{X}(0)\rangle} |I\rangle + \frac{x_\Pi(t)}{\langle \Pi |\bar{X}(0)\rangle} |\Pi\rangle \\
= |I\rangle \langle I | \bar{X}(0) \cos(\omega_1 t) + |\Pi\rangle \langle \Pi | \bar{X}(0) \cos(\omega_\Pi t)
\]

From this we can get \(x_1(t)\) and \(x_2(t)\) by projecting with \(\langle 1 |\) and \(\langle 2 |\) respectively:

\[
x_1(t) = \frac{\langle 1 | \bar{X}(t)\rangle}{\langle 1 | \bar{X}(0)\rangle} = \frac{\langle 1 | I \rangle \langle I | \bar{X}(0) \rangle \cos(\omega_1 t) + \langle 1 | \Pi \rangle \langle \Pi | \bar{X}(0) \rangle \cos(\omega_\Pi t)}{\langle 1 | \bar{X}(0)\rangle} \\
= \frac{1}{\omega_1} \left[ x_1(0) \cos(\omega_1 t) + x_\Pi(0) \cos(\omega_\Pi t) \right]
\]

\[
x_2(t) = \frac{\langle 2 | \bar{X}(t)\rangle}{\langle 2 | \bar{X}(0)\rangle} = \frac{\langle 2 | I \rangle \langle I | \bar{X}(0) \rangle \cos(\omega_1 t) + \langle 2 | \Pi \rangle \langle \Pi | \bar{X}(0) \rangle \cos(\omega_\Pi t)}{\langle 2 | \bar{X}(0)\rangle} \\
= \frac{1}{\omega_\Pi} \left[ x_1(0) \cos(\omega_1 t) - x_\Pi(0) \cos(\omega_\Pi t) \right]
\]
To complete we only need to express $X_1(0)$ and $X_2(0)$ in terms of $X_1(0)$ and $X_2(0)$:

$$X_\Pi(0) = \langle I \mid \vec{x}(0) \rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} X_1(0) \\ X_2(0) \end{pmatrix} = \frac{X_1(0) - X_2(0)}{\sqrt{2}}$$

$$X_\Pi(0) = \langle II \mid \vec{x}(0) \rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} X_1(0) \\ X_2(0) \end{pmatrix} = \frac{X_1(0) + X_2(0)}{\sqrt{2}}$$

$$\Rightarrow X_1(t) = \frac{X_1(0) + X_2(0)}{2} \cos(\omega_\Pi t) + \frac{X_1(0) - X_2(0)}{2} \cos(\omega_\Pi t)$$

$$X_2(t) = \frac{X_1(0) + X_2(0)}{2} \cos(\omega_\Pi t) - \frac{X_1(0) - X_2(0)}{2} \cos(\omega_\Pi t)$$

Or in matrix form:

$$\begin{pmatrix} X_1(t) \\ X_2(t) \end{pmatrix} = \begin{pmatrix} 1/2 \left[ \cos(\frac{\omega_\Pi}{m} t) + \cos(\frac{\omega_m}{m} t) \right] & \frac{1}{2} \left[ \cos(\frac{\omega_\Pi}{m} t) - \cos(\frac{\omega_m}{m} t) \right] \\ \frac{1}{2} \left[ \cos(\frac{\omega_\Pi}{m} t) - \cos(\frac{\omega_m}{m} t) \right] & 1/2 \left[ \cos(\frac{\omega_\Pi}{m} t) + \cos(\frac{\omega_m}{m} t) \right] \end{pmatrix} \begin{pmatrix} X_1(0) \\ X_2(0) \end{pmatrix}$$

---

Here is a summary of the steps:

1. Solve the eigenvalue problem for $\hat{H}$

2. Find $X_\Pi(0) = \langle I \mid \vec{x}(0) \rangle$ and $X_\Pi(0) = \langle II \mid \vec{x}(0) \rangle$ from the initial conditions.

   The initial state is $|\vec{x}(0)\rangle = |I\rangle X_1(0) + |II\rangle X_\Pi(0)$ (*).

3. To find the dependence $|\vec{x}(t)\rangle$, simply take the r.h.s. of (*) and multiply each coefficient $X_i(0)$ ($i = I, II$) by $\cos(\omega_i t)$

4. To find the positions $x_1(t)$ and $x_2(t)$ of the masses, project the solution on $|1\rangle$ and $|2\rangle$:

   $$(1 \mid \vec{x}(t)\rangle = x_1(t), \quad (2 \mid \vec{x}(t)\rangle = x_2(t)$$
The propagator

The solution of this problem has a remarkable structure:

1. The final state vector is obtained from the initial state vector by multiplication with a matrix, and this matrix is independent of the initial state.

This matrix is called the *propagator*.

We can view our solution as the representation in the \( |1\rangle, |2\rangle \) basis of the abstract relation

\[
|\hat{x}(t)\rangle = \hat{U}(t) |x(0)\rangle
\]

We read off from the underlined equation of \( p.41 \):

\[
\hat{U}(t) = |I\rangle \langle I| \cos(\omega t) + |II\rangle \langle II| \cos(\omega t) \\
= \sum_{i=1}^{2} |i\rangle \langle i| \cos(\omega_i t)
\]

This is a sum over projectors on the eigenvectors with weight \( \cos(\omega_i t) \). This structure is very generic and embodies the key features of time evolution also in quantum mechanics.

The matrix elements of \( \hat{U}(t) \) in the \( |1\rangle, |2\rangle \) basis are the matrix entries in the framed equation \( p.42 \).

So to solve the problem \( |\ddot{x}\rangle = \hat{\Sigma} |x\rangle \):

1. solve the eigenvalue problem of \( \hat{\Sigma} \)
2. construct the propagator \( \hat{U}(t) \) from eigenvectors and eigenvalues as in \( \S \)
3. write down \( |\hat{x}(t)\rangle = \hat{U}(t) |x(0)\rangle \). That's it!
The eigenkets $|\text{I}\rangle, |\text{II}\rangle$ are abstract vectors describing what in classical mechanics are called "normal modes". They evolve "trivially":

$$|\text{I}(t)\rangle = \cos(\omega_{\text{I}} t) \ |\text{I}\rangle$$
$$|\text{II}(t)\rangle = \cos(\omega_{\text{II}} t) \ |\text{II}\rangle$$

In the eigenbasis (normal mode representation) the propagator is diagonal:

$$\hat{U}(t) \leftrightarrow \begin{pmatrix} 
\cos(\omega_{\text{I}} t) & 0 \\
0 & \cos(\omega_{\text{II}} t)
\end{pmatrix}$$

The central problem in Quantum Mechanics is to solve the Schrödinger equation:

$$i \hbar \dot{|\psi\rangle} = \hat{H} \ |\psi\rangle \quad (t = \frac{\hbar}{2\pi})$$

$\hat{H}$ is called the Hamiltonian, $|\psi\rangle$ the state vector of the system. (All the conceptual complexities of QT have to do with how one computes physical observables from that state vector.)

The problem is to find $|\psi(t)\rangle$ given $|\psi(0)\rangle$.

This problem is formally very similar to the 2-oscillator problem we just solved:

1. Solve the eigenvalue problem of $\hat{H}$
2. Find the propagator $\hat{U}(t)$ in terms of eigenvectors and eigenvalues of $\hat{H}$.
3. $|\psi(t)\rangle = \hat{U}(t) \ |\psi(0)\rangle$. That's it!