(μ) Normal Operators

We assume that the properties of linear operators (endomorphisms) $\mathcal{H} \to \mathcal{H}$ in dimension $d > 0$ are well known, in particular the notions of determinant, diagonalization, eigenvalues, and eigenvectors.

Recall that for an operator $M : \mathcal{H} \to \mathcal{H}$, $|\psi\rangle \in \mathcal{H}$ is an **eigenvector** (nonzero) associated with the **eigenvalue** (or spectral value) $\lambda \in \mathbb{C}$ if $M|\psi\rangle = \lambda|\psi\rangle$. Every eigenvalue λ of M therefore provides a nonzero solution to the equation $(M-\lambda\mathbb{1})|\psi\rangle = 0$, which amounts to saying that the matrix $M - \lambda\mathbb{1}$ is not invertible, or equivalently that its determinant is zero: $|M-\lambda\mathbb{1}| = 0$. This determinant is a polynomial of degree d in λ, which has d complex roots. Consequently, the eigenvalues of M are uniquely determined by the operator M, as the roots of this polynomial. For this λ, the **eigenspace** $\mathcal{H}_\lambda$ is the subspace of $\mathcal{H}$ consisting of all vectors solving the equation $M|\psi\rangle = \lambda|\psi\rangle$, that is, the kernel $\mathrm{Ker}(M - \lambda\mathbb{1})$, which is also uniquely determined by M.

In quantum theory, we consider only normal operators in the following sense.

Definition. *A (linear) operator $M : \mathcal{H} \to \mathcal{H}$ is **normal** if it is diagonalizable in an orthonormal basis $|a\rangle$.*

The orthonormal basis $|a\rangle$ $(a \in A)$ is the basis of eigenvectors associated with the eigenvalues $\lambda_a \in \mathbb{C}$ of M, which are the diagonal entries of M written in this basis. According to the general expression of a matrix $M = \sum_{a,b} M_{a,b}|a\rangle\langle b|$, the only nonzero entries are the $M_{a,a} = \lambda_a$, and saying that M is normal amounts to saying that it can be written in **spectral decomposition** form:

$$M = \sum_a \lambda_a \, |a\rangle\langle a|$$

where the sum runs over the $d = \dim\mathcal{H}$ elements of A.

The eigenvalues λ_a are uniquely determined by M but are not necessarily distinct; there may be multiple eigenvalues. By writing $|\psi\rangle$ in the basis of the $|a\rangle$, one finds that the solutions of the equation $M|\psi\rangle = \lambda|\psi\rangle$ are the vectors spanned by the $|a\rangle$ for all $a \in A$ such that $\lambda_a = \lambda$. These therefore form an orthonormal basis of the eigenspace $\mathcal{H}_\lambda$, and the multiplicity of the eigenvalue λ is equal to its dimension $\dim\mathcal{H}_\lambda$.

By grouping the terms with the same eigenvalues in the expression $\sum_a \lambda_a \, |a\rangle\langle a| = \sum_\lambda \lambda(\sum_{a|\lambda_a=\lambda} |a\rangle\langle a|)$, one obtains the **canonical spectral decomposition**:

$$M = \sum_\lambda \lambda \, \Pi_\lambda$$

whose elements are uniquely determined by M: the sum ranges over the set of eigenvalues (the **spectrum**) of M, and Π_λ is the orthogonal projector $\Pi_\lambda = \sum_{a|\lambda_a=\lambda} |a\rangle\langle a|$ onto the eigenspace $\mathcal{H}_\lambda$, called the **spectral projector** associated with λ.

Remark. By comparison, in the spectral decomposition $M = \sum_a \lambda_a |a\rangle\langle a|$, the orthonormal eigenvectors $|a\rangle$ are not unique, because they depend on the choice of orthonormal bases for each eigenspace. Even for a simple eigenvalue λ_a for which $\dim \mathcal{H}_{\lambda_a} = 1$, the corresponding eigenvector $|a\rangle$ is determined only up to a phase (in quantum theory, this corresponds to the same state).

The canonical spectral decomposition may be viewed as a generalization of the resolution-of-the-identity formula, corresponding to the case $M = \mathbb{1}$, for which all eigenvalues are equal to 1:

$$\sum_\lambda \Pi_\lambda = \mathbb{1}$$

Moreover, since the bases of the eigenspaces $\mathcal{H}_\lambda$, that is, the $|a\rangle$ for which $\lambda_a = \lambda$, are disjoint subsets of the orthonormal basis of the $|a\rangle$ for the whole space $\mathcal{H}$, these eigenspaces are mutually orthogonal and we have the relations

$$\Pi_\lambda \Pi_{\lambda'} = \begin{cases} \Pi_\lambda & \text{if } \lambda = \lambda'; \\ 0 & \text{if } \lambda \neq \lambda'. \end{cases}$$

Thus, saying that M is normal amounts to saying that it can be decomposed in the form $M = \sum_\lambda \lambda\, \Pi_\lambda$, where the spectral projectors satisfy the two conditions above: $\sum_\lambda \Pi_\lambda = \mathbb{1}$ and $\Pi_\lambda \Pi_{\lambda'} = 0$ if $\lambda \neq \lambda'$.

Thanks to these properties, we will easily be able to compute matrix products of the form

$$\Big(\sum_\lambda f(\lambda)\, \Pi_\lambda\Big)\Big(\sum_\lambda g(\lambda)\, \Pi_\lambda\Big) = \sum_{\lambda',\lambda} f(\lambda')g(\lambda)\, \Pi_{\lambda'}\Pi_\lambda = \sum_\lambda f(\lambda)g(\lambda)\, \Pi_\lambda$$

which amount to performing the products on the eigenvalues.

The point of the notion of a normal operator is that it makes it easy to translate properties of an operator M into properties of the corresponding complex numbers (eigenvalues) λ. For example, the dual M^* corresponds to the conjugate eigenvalues λ^*, because by taking the conjugate transpose of the canonical spectral decomposition, we get

$$M^* = \sum_\lambda \lambda^*\, \Pi_\lambda^* = \sum_\lambda \lambda^*\, \Pi_\lambda$$

since every orthogonal projector is its own dual ($\Pi_\lambda^* = \Pi_\lambda$). Thus M^* is diagonalizable in the same orthonormal basis as M, with conjugate eigenvalues λ^*.

An important criterion for normality is given by the **spectral theorem**:

Theorem (spectral). *M is normal (diagonalizable in an orthonormal basis) if and only if it commutes with its dual:*

$$MM^* = M^*M$$

(This commutativity relation is often taken as the definition of a normal operator.)

Proof. First, if $M = \sum_\lambda \lambda\,\Pi_\lambda$ is normal, then $M^* = \sum_\lambda \lambda^*\,\Pi_\lambda$ and, by the properties of spectral projectors,

$$MM^* = \sum_\lambda \lambda\lambda^*\,\Pi_\lambda$$

Since $\lambda\lambda^* = |\lambda|^2 = \lambda^*\lambda$, the same calculation with the roles of M and M^* interchanged gives the relation $MM^* = M^*M$.

Conversely, assume that $MM^* = M^*M$, and consider an eigenvalue λ of M and the corresponding eigenspace $\mathcal{H}_\lambda$. The eigenspace $\mathcal{H}_\lambda$ is invariant under M since $|\psi\rangle \in \mathcal{H}_\lambda \implies M|\psi\rangle = \lambda|\psi\rangle \in \mathcal{H}_\lambda$. But, under the hypothesis $MM^* = M^*M$, it is also invariant under M^*, because $|\psi\rangle \in \mathcal{H}_\lambda \implies MM^*|\psi\rangle = M^*M|\psi\rangle = \lambda M^*|\psi\rangle \implies M^*|\psi\rangle \in \mathcal{H}_\lambda$.

Let Π_λ be the orthogonal projector onto $\mathcal{H}_\lambda$, and let $\Pi_\lambda^\perp = \mathbb{1} - \Pi_\lambda$ be the orthogonal projector onto the orthogonal complement $\mathcal{H}_\lambda^\perp$, so that we have the orthogonality relations $\Pi_\lambda\Pi_\lambda^\perp = \Pi_\lambda^\perp\Pi_\lambda = 0$. Since $\mathcal{H}_\lambda$ is invariant under M, with $M\Pi_\lambda = \lambda\Pi_\lambda$, we have $\Pi_\lambda^\perp M\Pi_\lambda = 0$. Moreover, since $\mathcal{H}_\lambda$ is invariant under M^*, we also have $\Pi_\lambda^\perp M^*\Pi_\lambda = 0$, whence, by taking the dual, $\Pi_\lambda M\Pi_\lambda^\perp = 0$; this amounts to saying that $\mathcal{H}_\lambda^\perp$ is also invariant under M. Consequently, the two cross terms vanish in the expansion

$$M = \mathbb{1}M\mathbb{1} = (\Pi_\lambda + \Pi_\lambda^\perp)M(\Pi_\lambda + \Pi_\lambda^\perp) = \Pi_\lambda M\Pi_\lambda + \Pi_\lambda^\perp M\Pi_\lambda + \Pi_\lambda M\Pi_\lambda^\perp + \Pi_\lambda^\perp M\Pi_\lambda^\perp$$

and what remains is

$$M = \lambda\,\Pi_\lambda + M'$$

where the operator $M' = \Pi_\lambda^\perp M\Pi_\lambda^\perp$ describes the restriction of M to the orthogonal complement $\mathcal{H}_\lambda^\perp$. Again, thanks to the vanishing of the cross terms $\Pi_\lambda^\perp M\Pi_\lambda = \Pi_\lambda M\Pi_\lambda^\perp = 0$, we get

$$\begin{aligned}
M'M'^* &= \Pi_\lambda^\perp M\Pi_\lambda^\perp M^*\Pi_\lambda^\perp = \Pi_\lambda^\perp M(\mathbb{1} - \Pi_\lambda)M^*\Pi_\lambda^\perp = \Pi_\lambda^\perp MM^*\Pi_\lambda^\perp \\
M'^*M' &= \Pi_\lambda^\perp M^*\Pi_\lambda^\perp M\Pi_\lambda^\perp = \Pi_\lambda^\perp M^*(\mathbb{1} - \Pi_\lambda)M\Pi_\lambda^\perp = \Pi_\lambda^\perp M^*M\Pi_\lambda^\perp
\end{aligned}$$

so the operator M' satisfies the same commutativity relation as M: $M'M'^* = M'^*M'$. We can therefore proceed with M' in the same way as with M, using an eigenvalue $\lambda' \neq \lambda$, to obtain the decomposition $M = \lambda\,\Pi_\lambda + \lambda'\,\Pi_{\lambda'} + M''$, and so on, until all eigenvalues of M are exhausted and its canonical spectral decomposition is obtained; this proves that M is normal. □

Definition. *The operator M is **Hermitian** (or self-adjoint) if it is self-dual: $M^* = M$.*

A Hermitian operator is normal, because by the spectral theorem $MM^* = M^2 = M^*M$. The spectral decompositions $M = \sum_\lambda \lambda\,\Pi_\lambda = M^* = \sum_\lambda \lambda^*\,\Pi_\lambda$ are equal if and only if the diagonal entries satisfy $\lambda = \lambda^*$, that is, $\lambda \in \mathbb{R}$: all eigenvalues are real. We therefore have the following.

Theorem (spectral, Hermitian case). *M is Hermitian if and only if it is normal (diagonalizable in an orthonormal basis) with real eigenvalues.*

Remark. Analogously, an operator M is **anti-Hermitian** if $M^* = -M$, which amounts to saying that it is a normal operator (diagonalizable in an orthonormal basis) whose eigenvalues are purely imaginary (because $\lambda^* = -\lambda \iff \lambda \in i\mathbb{R}$). One can always decompose an arbitrary operator (even a non-normal one) into Hermitian and anti-Hermitian parts:

$$M = \tfrac{1}{2}(M + M^*) + \tfrac{1}{2}(M - M^*)$$

where $\frac{1}{2}(M + M^*)$ is Hermitian and $\frac{1}{2}(M - M^*)$ is anti-Hermitian.

Definition. *The* ***Hermitian form*** *associated with the operator M is the map $\mathcal{H} \to \mathbb{C}$ defined by $\langle\psi|M|\psi\rangle$ for every $\psi \in \mathcal{H}$.*

It is clear that the sesquilinear form $\langle\phi|M|\psi\rangle$ (for all $\phi, \psi \in \mathcal{H}$) determines M uniquely, since in particular one recovers the matrix entries $\langle a|M|b\rangle$ in an orthonormal basis. It is important to observe that the Hermitian form alone, $\langle\psi|M|\psi\rangle$ (for every $\psi \in \mathcal{H}$), also determines the operator M uniquely. For this, it suffices to show that $\langle\psi|M|\psi\rangle = 0$ for every $\psi \in \mathcal{H}$ implies $M = 0$, because then, for two arbitrary operators M and N, the identity $\langle\psi|M|\psi\rangle = \langle\psi|N|\psi\rangle$ amounts to saying that $\langle\psi|(M - N)|\psi\rangle = 0$ for every $\psi \in \mathcal{H}$, whence $M - N = 0$ and $M = N$.

The property $\langle\psi|M|\psi\rangle = 0$ $(\forall\psi \in \mathcal{H}) \implies M = 0$ is true if M is normal, because then, in an orthonormal basis $|a\rangle$ of eigenvectors, $\lambda_a = \langle a|M|a\rangle = 0$ for every a implies $M = 0$. Otherwise, since $\langle\psi|M|\psi\rangle = 0$ implies $\langle\psi|M^*|\psi\rangle = \big(\langle\psi|M|\psi\rangle\big)^* = 0$, we get $\langle\psi|(M \pm M^*)|\psi\rangle = 0$ for every $\psi \in \mathcal{H}$, which implies $M \pm M^* = 0$ because the Hermitian and anti-Hermitian parts of M are normal. Hence finally $M = \frac{1}{2}(M + M^*) + \frac{1}{2}(M - M^*) = 0$. We have proved the following.

Theorem. *The Hermitian form $\langle\psi|M|\psi\rangle$ (for every $\psi \in \mathcal{H}$) determines an arbitrary operator M uniquely.*

In particular, M is Hermitian if and only if, for every $\psi \in \mathcal{H}$, $\langle\psi|M|\psi\rangle = \langle\psi|M^*|\psi\rangle$, that is, $\langle\psi|M|\psi\rangle = \big(\langle\psi|M|\psi\rangle\big)^*$, or equivalently $\langle\psi|M|\psi\rangle \in \mathbb{R}$:

Theorem. *M is Hermitian if and only if its Hermitian form is real-valued: $\langle\psi|M|\psi\rangle \in \mathbb{R}$ for every $\psi \in \mathcal{H}$.*

Remark. Analogously, M is anti-Hermitian if and only if its Hermitian form is purely imaginary: $\langle\psi|M|\psi\rangle \in i\mathbb{R}$ for every $\psi \in \mathcal{H}$.

Definition (Positivity and Löwner order). *The operator M is* ***positive*** *(or non-negative, equivalently positive semidefinite) if $\langle\psi|M|\psi\rangle \geqslant 0$ for every $\psi \in \mathcal{H}$. We then write $M \geqslant 0$.*

It is ***positive definite*** *if $\langle\psi|M|\psi\rangle > 0$ for every nonzero $\psi \in \mathcal{H}$. We then write $M > 0$.*
For convenience, for arbitrary Hermitian operators M, N, one often uses the ***Löwner notation*** *$M \geqslant N$ (or $N \leqslant M$), which means $M - N \geqslant 0$ and defines a partial order. Similarly, $M > N$ (or $N < M$) if $M - N > 0$.*

Remark. By replacing $|\psi\rangle$ by $N|\psi\rangle$ in the definitions above, one establishes that, for any operator N, if M is Hermitian then N^*MN is also Hermitian, and $M \geqslant 0 \implies N^*MN \geqslant 0$.

Since $\langle\psi|M|\psi\rangle \geqslant 0$ implies $\langle\psi|M|\psi\rangle \in \mathbb{R}$, a positive (or positive definite) operator is Hermitian, with eigenvalues $\lambda_a = \langle a|M|a\rangle$ that are nonnegative (respectively strictly positive):

Theorem (spectral, positive case). *M is positive semidefinite if and only if it is normal (diagonalizable in an orthonormal basis) with nonnegative eigenvalues $\lambda \geqslant 0$.*

M is positive definite if and only if it is normal (diagonalizable in an orthonormal basis) with strictly positive eigenvalues $\lambda > 0$.

Remark. Even if M is not normal (and even if it is a rectangular matrix), the two operators M^*M and MM^* are always positive semidefinite, since $\langle\psi|M^*M|\psi\rangle = \langle M\psi|M\psi\rangle = \|M\psi\|^2 \geqslant 0$ and $\langle\psi|MM^*|\psi\rangle = \langle M^*\psi|M^*\psi\rangle = \|M^*\psi\|^2 \geqslant 0$.

Remark. An orthogonal projector Π already constitutes its own spectral decomposition $\Pi = 0 \cdot \Pi_0 + 1 \cdot \Pi_1$, where $\Pi_1 = \Pi$ and $\Pi_0 = \mathbb{1} - \Pi$ is the projector onto the orthogonal complement. Since the eigenvalues are $\lambda = 0$ or $\lambda = 1$, Π is a positive Hermitian operator ($\Pi^* = \Pi$), satisfying $\Pi^2 = \Pi$. Conversely, every normal operator M satisfying $M = M^2$ is such that $\sum_\lambda \lambda\,\Pi_\lambda = \sum_\lambda \lambda^2\,\Pi_\lambda$, whence $\lambda = \lambda^2$, that is, $\lambda = 0$ or $\lambda = 1$.

Thus every **orthogonal projector** is characterized by being **normal** and **idempotent** (equal to its square).

We have established that the spectral projectors Π_λ in a spectral decomposition satisfy the relations $\sum_\lambda \Pi_\lambda = \mathbb{1}$ and $\Pi_\lambda\Pi_{\lambda'} = 0$ if $\lambda \neq \lambda'$. The second condition is in fact a consequence of the first. Indeed, assume that $\sum_\lambda \Pi_\lambda = \mathbb{1}$, and consider two projectors Π_λ and $\Pi_{\lambda'}$, where $\lambda \neq \lambda'$. Then $\Pi_{\lambda'} \geqslant 0$, and $\Pi_\lambda + \Pi_{\lambda'} \leqslant \mathbb{1}$ (because the difference is a sum of orthogonal projectors). Multiplying on the left and on the right by Π_λ, we obtain $\Pi_\lambda\Pi_{\lambda'}\Pi_\lambda \geqslant 0$, but also $\Pi_\lambda^3 + \Pi_\lambda\Pi_{\lambda'}\Pi_\lambda \leqslant \Pi_\lambda^2$, which simplifies to $\Pi_\lambda\Pi_{\lambda'}\Pi_\lambda \leqslant 0$ since $\Pi_\lambda = \Pi_\lambda^2$. Thus $\Pi_\lambda\Pi_{\lambda'}\Pi_\lambda = \Pi_\lambda^*\Pi_{\lambda'}^*\Pi_{\lambda'}\Pi_\lambda = 0$, that is, for every $|\psi\rangle$, $\langle\psi|\Pi_\lambda^*\Pi_{\lambda'}^*\Pi_{\lambda'}\Pi_\lambda|\psi\rangle = \|\Pi_{\lambda'}\Pi_\lambda\psi\|^2 = 0$, whence $\Pi_\lambda\Pi_{\lambda'} = 0$. We have proved the following theorem.

Theorem (orthogonal resolution of the identity). *If a family of orthogonal projectors sums to the identity, $\sum_\lambda \Pi_\lambda = \mathbb{1}$, then $\Pi_\lambda\Pi_{\lambda'} = 0$ for every $\lambda \neq \lambda'$.*

Thus, as soon as we have a resolution of the identity (closure relation) $\sum_\lambda \Pi_\lambda = \mathbb{1}$, the projectors Π_λ are necessarily projectors onto orthogonal subspaces, and there can be at most as many of them as the dimension d of $\mathcal{H}$. Consequently, the number of such projectors cannot exceed the dimension of the space.

Definition. *The operator U is **unitary** if it is invertible and its inverse is its dual:*

$$U^{-1} = U^*.$$

A unitary operator is normal, by the spectral theorem, because $UU^* = \mathbb{1} = U^*U$. Conversely, if $UU^* = \mathbb{1}$, then taking determinants gives $\det(U)\det(U^*) = |\det(U)|^2 = 1$, so U is invertible and $U^{-1} = U^{-1}UU^* = U^*$: U is unitary. Similarly, the relation $U^*U = \mathbb{1}$ implies that U is unitary. The three conditions $UU^* = \mathbb{1}$, $U^*U = \mathbb{1}$, and $U^{-1} = U^*$ are therefore equivalent.

The product of the spectral decompositions $U = \sum_\lambda \lambda\,\Pi_\lambda$ and $U^* = \sum_\lambda \lambda^*\,\Pi_\lambda$ gives $UU^* = \sum_\lambda \lambda\lambda^*\,\Pi_\lambda = \sum_\lambda |\lambda|^2\,\Pi_\lambda$. Consequently, U is unitary if and only if it is normal with eigenvalues satisfying $|\lambda| = 1$ (in other words, $\lambda \in \mathbb{U}$, where $\mathbb{U}$ denotes the unit circle of $\mathbb{C}$).

Theorem (spectral, unitary case). *U is unitary if and only if it is normal (diagonalizable in an orthonormal basis) with eigenvalues of modulus 1.*

By the characterization of the associated Hermitian form, U is unitary if and only if $\langle\psi|U^*U|\psi\rangle = \langle\psi|\mathbb{1}|\psi\rangle = \langle\psi|\psi\rangle$, that is, $\|U\psi\|^2 = \|\psi\|^2$ for every $\psi \in \mathcal{H}$:

Theorem. *U is unitary if and only if it preserves the norm: $\|U\psi\| = \|\psi\|$ for every $\psi \in \mathcal{H}$.*

More generally, it preserves the inner product, because for all $\phi, \psi \in \mathcal{H}$, $\langle U\phi|U\psi\rangle = \langle\phi|U^*U|\psi\rangle = \langle\phi|\mathbb{1}|\psi\rangle = \langle\phi|\psi\rangle$.

Remark. If the $|i\rangle$ (say for $i = 1, \ldots, d$) denote the vectors of the canonical orthonormal basis, the condition $U^*U = \mathbb{1}$ amounts to saying that

$$\langle Ui|Uj\rangle = \langle i|U^*U|j\rangle = \begin{cases} 1 & \text{if } i = j; \\ 0 & \text{otherwise.} \end{cases}$$

In other words, the d **columns** $U|j\rangle$ of the matrix U are **orthonormal**. Similarly, the condition $UU^* = \mathbb{1}$ amounts to saying that the d **rows** $\langle i|U$ of the matrix U are **orthonormal**.

Thus the vectors $|u_i\rangle = U|i\rangle$ form a new orthonormal basis, in which the matrix of an arbitrary operator M is the matrix of coefficients

$$\langle u_i|M|u_j\rangle = \langle Ui|M|Uj\rangle = \langle i|U^*MU|j\rangle\,.$$

This amounts to saying that the matrix of the operator M in the new orthonormal basis of the $|u_i\rangle$ is equal to U^*MU.

In particular, M is normal if and only if there exists a unitary operator U such that $U^*MU = \Lambda$ is diagonal, where the diagonal entries are the eigenvalues λ_i associated with the eigenvectors $|u_i\rangle$:

$$U^*MU = \Lambda = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & 0 \\ & & \ddots & \\ 0 & & & \lambda_d \end{pmatrix}$$

Since $U^{-1} = U^*$, we can invert the relation: $M = U\Lambda U^*$, which is equivalent to the spectral decomposition $M = \sum_i \lambda_i |u_i\rangle\langle u_i|$.

The following table summarizes the different types of operators:

normal	$MM^* = M^*M$	$\lambda\lambda^* = \lvert\lambda\rvert^2 = \lambda^*\lambda$	$\lambda \in \mathbb{C}$
unitary	$MM^* = M^*M = \mathbb{1}$	$\lvert\lambda\rvert^2 = 1$	$\lambda \in \mathbb{U}$
Hermitian	$M^* = M$	$\lambda^* = \lambda$	$\lambda \in \mathbb{R}$
anti-Hermitian	$M^* = -M$	$\lambda^* = -\lambda$	$\lambda \in i\mathbb{R}$
positive	$M \geqslant 0$	$\lambda \geqslant 0$	$\lambda \in \mathbb{R}_+$
positive definite	$M > 0$	$\lambda > 0$	$\lambda \in \mathbb{R}_+^*$
projector	$M^2 = M$	$\lambda^2 = \lambda$	$\lambda \in \{0, 1\}$

We can pursue the analogy between a normal operator and the set of its eigenvalues for any functional calculus on an operator, thanks to the following definition:

Definition. *For every normal operator $M = \sum_\lambda \lambda\, \Pi_\lambda$, and for every real- or complex-valued function f whose domain contains the eigenvalues $\lambda \in \mathbb{C}$, we define*

$$f(M) = \sum_\lambda f(\lambda)\, \Pi_\lambda.$$

This notation is compatible with the usual notation for operators, for example:

$f(\lambda) = \lambda^*$: $f(M) = \sum_\lambda \lambda^*\, \Pi_\lambda = M^*$ is the dual of M;

$f(\lambda) = \lambda^2$: $f(M) = \sum_\lambda \lambda^2\, \Pi_\lambda = (\sum_\lambda \lambda\, \Pi_\lambda)^2 = M^2$ is the usual square of M;

$f(\lambda) = \lambda^n$: $f(M) = \sum_\lambda \lambda^n\, \Pi_\lambda = (\sum_\lambda \lambda\, \Pi_\lambda)^n = M^n$ (calculation by induction) is the nth power of M;

$f(\lambda)$ **a polynomial in** λ: by linearity, $f(M)$ is the corresponding polynomial in M;

$f(\lambda) = \lambda^{-1}$: $f(M) = \sum_\lambda \lambda^{-1}\, \Pi_\lambda = M^{-1}$ is the inverse of M (if M is invertible, that is, if no eigenvalue is zero), because $MM^{-1} = \sum_\lambda \lambda\lambda^{-1}\, \Pi_\lambda = \mathbb{1}$.

We can also recover other definitions:

$f(\lambda) = \mathrm{Re}(\lambda) = \frac{1}{2}(\lambda + \lambda^*)$: $\mathrm{Re}(A) = \frac{1}{2}(A + A^*)$ is the Hermitian part of A.

$f(\lambda) = i\,\mathrm{Im}(\lambda) = \frac{1}{2}(\lambda - \lambda^*)$: $i\,\mathrm{Im}(A) = \frac{1}{2}(A - A^*)$ is the anti-Hermitian part of A (so $\mathrm{Im}(A)$ is Hermitian).

$f(\lambda) = \sqrt{\lambda}$: If $M \geqslant 0$, $\sqrt{M} = \sum_\lambda \sqrt{\lambda}\, \Pi_\lambda$ is the positive square root of M, which satisfies $\sqrt{M} \geqslant 0$ and $(\sqrt{M})^2 = M$.

$f(\lambda) = |\lambda| = \sqrt{\lambda\lambda^*}$: $|M| = \sqrt{MM^*} = \sqrt{M^*M} = \sum_\lambda |\lambda|\, \Pi_\lambda$ is the absolute value of M, which is positive: $|M| \geqslant 0$.

$f(\lambda) = \exp(\lambda)$: $\exp(M) = \sum_\lambda \exp(\lambda)\, \Pi_\lambda$, which we write as e^M in the natural base e. One can check that this definition coincides with the exponential of the matrix M defined by a series expansion.

$f(\lambda) = e^{i\lambda}$: If M is Hermitian, $e^{iM} = \sum_\lambda e^{i\lambda}\, \Pi_\lambda$ is unitary.
Conversely, a unitary operator $U = \sum_\lambda \lambda\, \Pi_\lambda$, where $\lambda = e^{i\theta} \in \mathbb{U}$, can be written in the form

$$U = e^{i\Theta}$$

where $\Theta = \sum_\theta \theta\, \Pi_\theta$ is Hermitian (each spectral projector Π_λ coincides with the corresponding spectral projector Π_θ, the eigenspaces being identical).

$f(\lambda) = \log\lambda$: If $M > 0$, $\log M = \sum_\lambda \log\lambda\, \Pi_\lambda$, written $\ln M$ in the natural base, is Hermitian. The matrix logarithm $\log M$ ($M > 0$) satisfies the identities $\log(M^{-1}) = -\log M$ and $\exp\log M = M$. If M is Hermitian, we also have $\exp M > 0$ and $\log\exp M = M$.

$f(\lambda) = \mathbb{1}_E(\lambda) = \mathbb{1}_{\lambda\in E}$: (indicator function of the set E): $\mathbb{1}_E(M) = \sum_{\lambda\in E} \Pi_\lambda$ is also called a **spectral projector**, and coincides with Π_λ if the set E reduces to the singleton $\{\lambda\}$. For notational convenience, we may write $\mathbb{1}_E(M) = \mathbb{1}_{M\in E}$.

If $E = \mathbb{C}$, we recover the resolution of the identity $\mathbb{1}$ for the constant function f equal to 1, which justifies the notation $\mathbb{1}$ for the identity operator.

$f(\lambda) = \operatorname{sgn}\lambda$: If M is Hermitian, $\operatorname{sgn} M = \sum_\lambda \operatorname{sgn}\lambda\, \Pi_\lambda$ is the sign of M, which is the difference of the two spectral projectors $\operatorname{sgn} M = \mathbb{1}_{M>0} - \mathbb{1}_{M<0}$. We have the relations $M = |M| \operatorname{sgn} M$, $|M| = M \operatorname{sgn} M$, and, for invertible M, $\operatorname{sgn} M = |M|^{-1}M = M|M|^{-1} = |M|M^{-1} = M^{-1}|M|$.

$f(\lambda) = \lambda^+ = \max(\lambda, 0)$, $f(\lambda) = \lambda^- = \max(-\lambda, 0)$: If M is Hermitian, its **positive and negative parts** $M^+ = M\mathbb{1}_{M>0}$ and $M^- = -M\mathbb{1}_{M<0}$ are positive operators. We have the decompositions $M = M^+ - M^-$ (sometimes called the **Hahn–Jordan decomposition**) and $|M| = M^+ + M^-$.

In all these examples, operators of the form $f(M)$, $g(M)$, etc. are simultaneously diagonalizable in the same orthonormal basis, and therefore they commute pairwise, since

$$f(M)g(M) = \sum_\lambda f(\lambda)g(\lambda)\,\Pi_\lambda = \sum_\lambda g(\lambda)f(\lambda)\,\Pi_\lambda = g(M)f(M).$$

So far, all the operators considered have involved only a single operator M, but this type of calculation can be generalized to the case of several normal operators M_i, where i ranges over an index set I. We have the following important result:

Theorem (simultaneous diagonalization). *The normal operators M_i $(i \in I)$ are simultaneously diagonalizable in the same orthonormal basis:*

$$M_i = \sum_\lambda m_{i,\lambda}\,\Pi_\lambda. \qquad (\forall i \in I)$$

if and only if they commute pairwise: $M_iM_j = M_jM_i$ for all $i, j \in I$.

Proof. Suppose that $M_i = \sum_\lambda m_{i,\lambda}\,\Pi_\lambda$ for every i, where the $m_{i,\lambda}$ denote the eigenvalues of M_i. Then, by the properties of spectral projectors,

$$M_iM_j = \sum_{\lambda',\lambda} m_{i,\lambda'}m_{j,\lambda}\,\Pi_{\lambda'}\Pi_\lambda = \sum_\lambda m_{i,\lambda}m_{j,\lambda}\Pi_\lambda.$$

Since $m_{i,\lambda}m_{j,\lambda} = m_{j,\lambda}m_{i,\lambda}$, the same calculation with the roles of i and j interchanged gives the commutation relation $M_iM_j = M_jM_i$. Notice that each eigenspace $\mathcal{H}_\lambda$ in these spectral decompositions is common to all the M_i, and is therefore invariant under all the M_i.

Conversely, suppose that $M_iM_j = M_jM_i$ for all i, j. The whole space $\mathcal{H}$ is obviously invariant under all the M_i, but we may consider a subspace $\mathcal{H}'$ of $\mathcal{H}$ that is invariant under all the M_i and has *minimal* dimension $d' > 0$ (such a subspace $\mathcal{H}'$ need not be unique). For each i, we may consider the restriction of M_i to $\mathcal{H}'$, which is an operator $\mathcal{H}' \to \mathcal{H}'$. This operator has an eigenvalue λ_i, and the corresponding eigenspace $\mathcal{H}_{\lambda_i} \subset \mathcal{H}'$ is invariant under M_i, since $|\psi\rangle \in \mathcal{H}_{\lambda_i} \implies M_i|\psi\rangle = \lambda_i|\psi\rangle \in \mathcal{H}_{\lambda_i}$. But, under the assumption $M_iM_j = M_jM_i$, it is also invariant under every M_j, for every j, because

$$|\psi\rangle \in \mathcal{H}_{\lambda_i} \implies M_iM_j|\psi\rangle = M_jM_i|\psi\rangle = \lambda_i M_j|\psi\rangle \implies M_j|\psi\rangle \in \mathcal{H}_{\lambda_i}.$$

Since $\mathcal{H}_{\lambda_i} \subset \mathcal{H}'$ is invariant under all the M_j, and $\mathcal{H}'$ has minimal dimension $d' > 0$ among the subspaces with this property, we necessarily have $\mathcal{H}' = \mathcal{H}_{\lambda_i}$, and this holds for every i.

Writing Π' for the orthogonal projector onto $\mathcal{H}'$, we can therefore write all the spectral decompositions of the M_i in the form

$$M_i = \lambda_i \Pi' + M_i'$$

for every i, where the same projector Π' is common to all these decompositions. Since these are spectral decompositions involving projectors onto mutually orthogonal spaces, the cross terms vanish: $\Pi' M_i' = M_i'\Pi' = 0$ for every i, and $M_iM_j = \lambda_i\lambda_j\Pi' + M_i'M_j'$ for all i, j. Consequently, the remaining operators M_i' (which represent the restrictions of the M_i to the orthogonal complement $\mathcal{H}'^{\perp}$) still commute pairwise. We may therefore proceed for the M_i' in the same way as for the M_i, to obtain the decomposition $M_i = \lambda_i\Pi' + \lambda_i'\Pi'' + M_i''$, and so on, until all the spectral decompositions of the M_i have been obtained with the same orthogonal projectors, that is, a simultaneous diagonalization of all the M_i in a single orthonormal basis. □

Example. If two normal operators M, N commute, they have simultaneous spectral decompositions

$$M = \sum_\lambda m_\lambda \Pi_\lambda \quad N = \sum_\lambda n_\lambda \Pi_\lambda.$$

It follows that $M + N$ and MN are also normal, with respective eigenvalues $m_\lambda + n_\lambda$ and $m_\lambda n_\lambda$, and we have, for example, the formulas $e^{M+N} = e^M e^N$ and, if $M, N > 0$, $\ln(MN) = \ln M + \ln N$.

More generally, if we have a finite number of normal operators A_i that commute pairwise, then

$$\exp \sum_i A_i = \prod_i \exp A_i$$
$$\log \prod_i A_i = \sum_i \log A_i \quad \text{if } A_i > 0 \text{ for every } i.$$

Remark (Uniqueness of the Hahn–Jordan decomposition). The decomposition $M = M^+ - M^-$ is the unique decomposition of a Hermitian matrix M as a difference of two positive semidefinite operators $M = P - Q$ $(P, Q \geqslant 0)$ such that $PQ = 0$. Indeed, we do have $M^+M^- = 0$; conversely, if $PQ = 0$ and $M = P - Q$, then also $QP = (PQ)^* = 0$, and therefore $MP = P^2 = PM$ and $MQ = -Q^2 = QM$: P and Q commute with M, and are diagonalizable in the same orthonormal basis of eigenvectors of M. For every eigenvalue λ of M, we then have the decomposition $\lambda = \lambda_P - \lambda_Q$ with $\lambda_P\lambda_Q = 0$, where $\lambda_P \geqslant 0$ and $\lambda_Q \geqslant 0$ are the respective eigenvalues of P and Q associated with the same eigenvector. It follows easily that $\lambda_P = \lambda^+$ and $\lambda_Q = \lambda^-$, whence $P = M^+$ and $Q = M^-$.

Example. We recover as a special case the situation where the operators are all functions of a single normal operator M:

$$M_i = f_i(M),$$

because, as we have already observed, the M_i have simultaneous spectral decompositions by definition of $f_i(M)$, and therefore commute pairwise.

In fact, this is the general case. If the M_i commute pairwise, write their simultaneous spectral decompositions in the form

$$M_i = \sum_\lambda m_{i,\lambda} \, \Pi_\lambda$$

and consider, for example, the normal operator

$$M = \sum_\lambda \lambda \, \Pi_\lambda,$$

where the values of λ are distinct in this sum (any other operator with distinct eigenvalues m_λ would do). We can then always find, for each index i, a function f_i such that

$$f_i(\lambda) = m_{i,\lambda} \qquad \text{for every } \lambda.$$

For example, we can define f_i as an interpolation polynomial of degree $< d$ (a Lagrange or Newton polynomial) that takes the value $m_{i,\lambda}$ at each distinct point λ (among at most $d = \dim \mathcal{H}$ distinct points). We then have $M_i = f_i(M)$ for every i. We have proved the following theorem.

Theorem (polynomial representation). *The normal operators M_i commute pairwise (equivalently, are simultaneously diagonalizable in the same orthonormal basis) if and only if they are functions of a single normal operator M:*

$$M_i = f_i(M),$$

where f_i may be chosen as a polynomial of degree $< d$ (whose coefficients depend on M_i).

Remark. This theorem and the preceding one are valid for an infinite family of operators M_i (even an uncountable family).

In particular, in the case of a single operator, every function $f(M)$ can be written as $f(M) = P(M)$, where P is a polynomial of degree $< d$ (which depends on M itself).