01_Operadores_en

September 23, 2025

Operators

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[1]:
```
import sys
sys.path.append('../')
import macro_tQ as tQ

import numpy as np
import scipy.linalg as la
from IPython.display import display,Markdown,Latex
import matplotlib.pyplot as plt
from qiskit.visualization import array_to_latex
```

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Operators and Matrices

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In a vector space, besides the vectors themselves, it is essential to understand the different ways in which they can be **transformed** into one another,

Linearity refers to the following property:

$$A : (\alpha|u\rangle + \beta|w\rangle) \quad \rightarrow \quad |v\rangle = \alpha A|u\rangle + \beta A|w\rangle$$

Example: An operator easy to visualize is the rotation operator in a plane. Given an angle $\theta \in (0, 2\pi)$, the operator $A = R(\theta)$ rotates any vector by an angle θ counterclockwise. A vector in the plane $\mathbf{u} = (u_1, u_2)$ is equivalent to the complex number $u = u_1 + iu_2$ in the complex plane $V = \mathbb{C}$.

Written in polar form, $u = |u|e^{i\phi}$, and we know that a rotation by an angle θ is equivalent to adding this angle to the phase:

$$v = R(\theta)u = |u|e^{i(\phi+\theta)} = |u|e^{i\phi}e^{i\theta} = u \cdot e^{i\theta}$$

Therefore, to rotate a complex number by an angle θ, it is enough to multiply it by the phase factor $e^{i\theta}$, which corresponds to the operator $R(\theta)$ in the vector space $V = \mathbb{C}$.

The fundamental property of a rotation is to keep the modulus invariant, $|v| = |u|$.

Exercise 1.3.1

Using the previous example, define a function R that receives a vector in the plane (u_1, u_2) and returns the vector (v_1, v_2) with components rotated by an angle θ.

Solution

“‘python def R(u1, u2, theta): u = u1 + u2*1j* $v = u$ np.exp(1j * theta) # u rotated by angle theta return v.real, v.imag

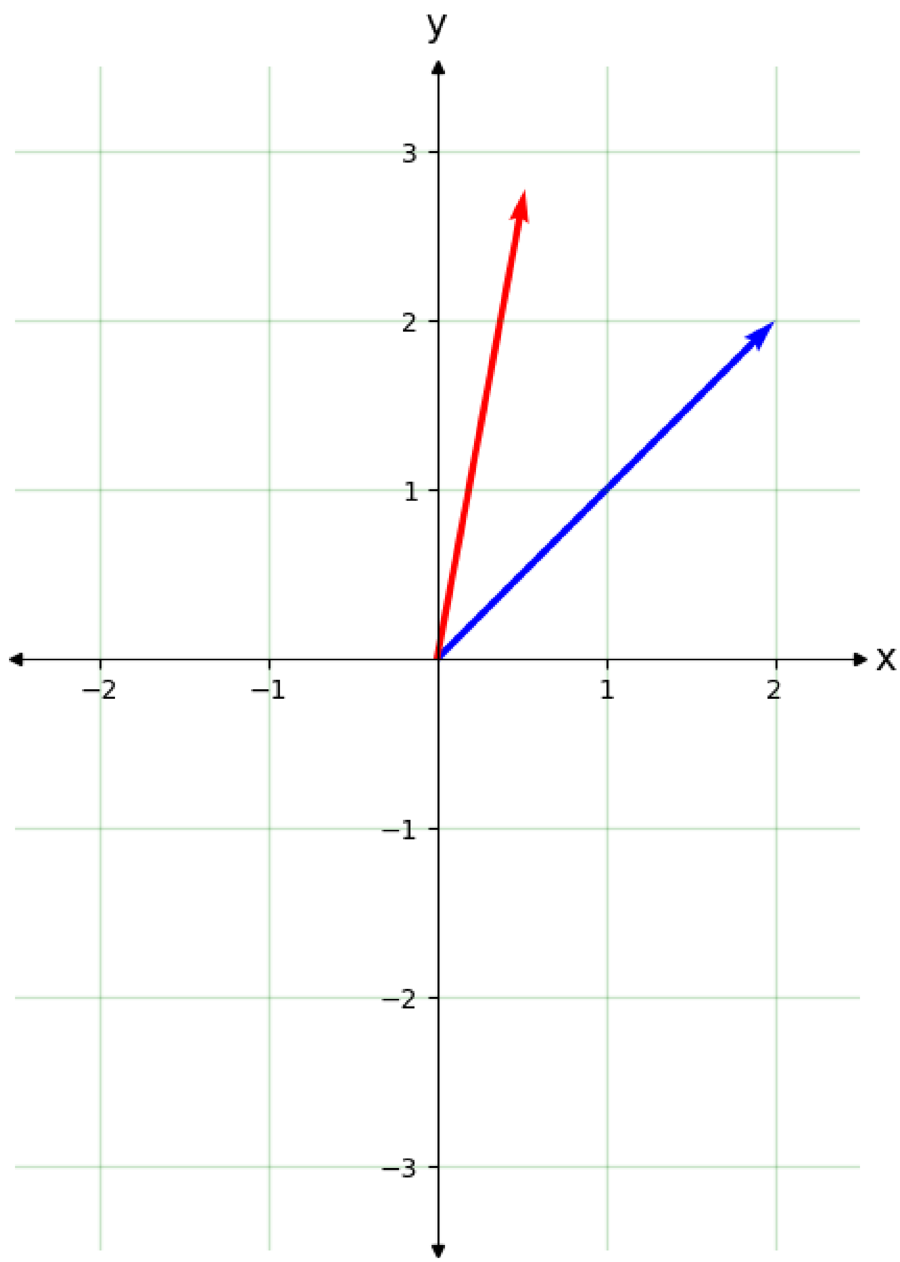
[3]:
```
'''ángulo que queremos rotar'''
theta=0.6

'''vector a rotar'''
u1=2.
u2=2.

'''v1 y v2 a partir de u1, u2 y theta'''
def R(u1,u2,theta):
        u = u1 + u2*1j
        v = u*np.exp(1j*theta) # u rotado un angulo theta
        return v.real,v.imag

v1,v2 =  R(u1,u2,theta)

''' Representación en el plano complejo '''
v = v1**2+v2**2
tQ.
 ↪plot_2D_plane(left=-int(abs(v1))-2,right=int(abs(v1))+2,up=int(abs(v2))+1,down=-int(abs(v2))-
tQ.draw_vector(u1,u1,vcolor='b')
tQ.draw_vector(v1,v2,vcolor='r')
```



0.1 Matrix of an operator

Given a basis $|i\rangle$

$\Rightarrow$ a vector is specified by a *column of components*

$$|v\rangle \sim \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}$$

$\Rightarrow$ an operator is defined by a *matrix of components.*

$$A \sim \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \cdots & A_{NN} \end{pmatrix}$$

Indeed, in a basis, the relation $|v\rangle = A|u\rangle$ is equivalent to an equation relating the components of both vectors.

$$v_i = \sum_{j=1}^{N} A_{ij}\ u_j\,.$$

This operation corresponds to the following matrix multiplication:

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \cdots & A_{NN} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix}$$

`<b>Example:</b>`

Continuing with the example of the rotation operator in a plane, we have seen that the components of $u = u_1 + iu_2$ and of $R(\theta)u = v = v_1 + iv_2$ are obtained by multiplication by a pure phase:

$$v = ue^{i\theta} \tag{1}$$
$$\tag{2}$$

Let's develop each side in Cartesian coordinates, separating the real and imaginary parts:

$$\begin{aligned} v_1 + iv_2 &= (u_1 + iu_2)(\cos\theta + i\sin\theta) && (3) \\ &= (\cos\theta\, u_1 - \sin\theta\, u_2) + i(\sin\theta\, u_1 + \cos\theta\, u_2) && (4) \end{aligned}$$

That is, the coordinates of the original vector and the rotated image vector are related as

$$v_1 = \cos\theta\, u_1 - \sin\theta\, u_2 \qquad , \qquad v_2 = \sin\theta\, u_1 + \cos\theta\, u_2 \tag{5}$$

which can be expressed in matrix form as

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

1 Basis of Operators

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Outer Product

Depending on the order in which we compose them, $\langle u|v\rangle$ or $|v\rangle\langle u|$, the result is very different

- The **inner product**, or *scalar product*, is a *complex number*

$$a = \langle u|v\rangle = \langle v|u\rangle^*$$

- The **outer product** is an *operator*

$$A = |v\rangle\langle u|$$

To understand why it is an operator, we observe that this expression applied to a vector $|w\rangle$ gives another vector,

$$A : |w\rangle \ \rightarrow \ A|w\rangle = |v\rangle\langle u|w\rangle = |v\rangle b = b|v\rangle$$

Note: 1. The order in which we write things is very important.
$\Rightarrow$ $\langle u|v\rangle$ and $|v\rangle\langle u|$ are radically different objects: the first is a number and the second is an operator.

$\Rightarrow$ On the other hand, $|v\rangle b = b|v\rangle$, as well as $\langle u|b = b\langle u|$, that is, complex numbers and *kets* or *bras* can be written in any order (we say they commute). 2. The action of the operator $A = |v\rangle\langle u|$ is very easy to describe in words:

- The operator A takes any vector $|w\rangle$ and converts it into a vector parallel to $|v\rangle$, proportional to its projection $b = \langle u|w\rangle$.

- If the projection is zero $b = 0$, the operator annihilates, that is, it gives the neutral element.

1.0.1 Outer product in components

The difference between the *inner product* $a = \langle u|v\rangle$ and the *outer product* $A = |u\rangle\langle v|$ is reflected in a basis by expressing both vectors, $|u\rangle = \sum_i u_i|i\rangle$ and $|v\rangle = \sum_j v_j|j\rangle$, in components in an orthonormal basis.

- The *complex number* a is the *scalar product*

$$a = \langle u|v\rangle = \left(u_1^*, ..., u_N^*\right) \begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix} = \sum_i u_i^* v_i$$

- The matrix A_{ij} *represents* the operator A in the basis $\{|i\rangle = |e_i\rangle\}$

$$
A = |v\rangle\langle u| \;\sim\; \begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix} \left(u_1^*, ..., u_N^*\right) \;=\; \begin{pmatrix} v_1 u_1^* & v_1 u_2^* & ... & v_1 u_N^* \\ v_2 u_1^* & v_2 u_1^* & ... & v_2 u_N^* \\ \vdots & \vdots & \ddots & \vdots \\ v_N u_1^* & & ... & v_N u_N^* \end{pmatrix} \;=\; A_{ij}
$$

Canonical basis of operators

Consider the *outer product* of two elements of the orthonormal basis $|i\rangle\langle j|$

- The action of $|i\rangle\langle j|$ on another vector, $|k\rangle$, of the basis is simple:

$$
|i\rangle\langle j|k\rangle = |i\rangle\delta_{jk} = \left\{ \begin{array}{ccc} 0 & \text{if} & k \neq j \\ |i\rangle & \text{if} & k = j \end{array} \right.
$$

- The matrix associated with the operator has only a 1 in the (i, j) element and zeros everywhere else. For example, suppose $N = 4$

$$
|2\rangle\langle 3| \;\rightarrow\; \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \Rightarrow \quad A_{ij} = \delta_{i2}\delta_{j3}
$$

The matrix elements A_{ij} express the components of an operator in the operator basis $|i\rangle\langle j|$.

$$
A \;=\; \sum_{i,j=1}^{N} A_{ij}|i\rangle\langle j|
$$

Consistency

Let's verify that it acts correctly

$$
\begin{aligned}
A|u\rangle \quad &= \quad \textstyle\sum_{i,j} A_{ij}|i\rangle\langle j| \left(\sum_k u_k|k\rangle\right) \\
&\overset{\text{linealidad}}{=} \quad \textstyle\sum_{i,j}\sum_k A_{ij}|i\rangle\, u_k\langle j|k\rangle \\
&\overset{\text{ortonormalidad}}{=} \quad \textstyle\sum_{i,j,k} A_{ij}|i\rangle\, u_k\delta_{jk} \\
&= \quad \textstyle\sum_{ij} A_{ij}\,|i\rangle\, u_j = \sum_i \left(\sum_j A_{ij}\, u_j\right)|i\rangle \\
&= \quad \textstyle\sum_i v_i|i\rangle \\
&= \quad |v\rangle
\end{aligned}
$$

1.0.2 Matrix elements

In the same way that we obtained the components of a vector by projecting onto a basis element

$$
v_i = \langle i|v\rangle
$$

we can now obtain the *matrix elements* of an operator A as

$$A_{ij} = \langle i|A|j\rangle$$

Exercise 1.3.2 Check the consistency of the expressions $\$\tilde{}\mathrm{A} = \sum \{i,j{=}1\}\hat{}N\ A\{ij\}|i\rangle\langle j|\$ and\ A_{ij} = \langle i|A|j\rangle$

Solution:

Here is your solution

Summary:
Given a basis $\{|i\rangle\}$, we can express an operator through a matrix A_{ij}. The precise relation is - as an operator $\rightarrow\ A = \sum_{ij} A_{ij}|i\rangle\langle j|$
- as a matrix element $\rightarrow\ A_{ij} = \langle i|A|j\rangle$

1.0.3 Change of basis

Two orthonormal bases $|e_i\rangle$ and $|\tilde{e}_i\rangle$ are linearly related by a matrix

$$|e_j\rangle \rightarrow |\tilde{e}_j\rangle = \sum_i U_{ij}|e_i\rangle$$

The *adjoint* relation is straightforward to obtain:

$$\langle e_j| \rightarrow \langle \tilde{e}_j| = \sum_i U^*_{ij}\langle e_i|$$

In each basis, an operator A is *represented* by different matrix elements

$$A_{ij} = \langle e_i|A|e_j\rangle \quad , \qquad \tilde{A}_{ij} = \langle \tilde{e}_i|A|\tilde{e}_j\rangle\,.$$

We can find the relation by substituting the change of basis

$$\begin{aligned}
\tilde{A}_{ij} &= \langle \tilde{e}_i|A|\tilde{e}_j\rangle && (6)\\
&= \sum_k U^*_{ki}\langle e_k|\ A\ \sum_l U_{lj}|e_l\rangle && (7)\\
&= \sum_{k,l} U^\dagger_{ik}\langle e_k|A|e_l\rangle U_{lj} = \sum_{k,l} U^\dagger_{ik} A_{kl} U_{lj}\,. && (8)
\end{aligned}$$

Lemma :
Under a change of orthonormal bases $\$\ |\mathrm{e}_j\rangle \rightarrow |\tilde{e}_j\rangle = \sum \{i\}\ U\{ij\}|e_i\rangle\$, thecomponentsofavector|v\rangle$ and of an operator A change according to the rule:

$$\begin{aligned} \tilde{v}_i &= (U^\dagger \cdot v)_i \qquad (9) \\ \tilde{A}_{ij} &= (U^\dagger \cdot A \cdot U)_{ij} \qquad (10) \end{aligned}$$

Note:
The mnemonic rule is that columns are multiplied by $U^\dagger \cdot$ and rows by $\cdot U$

$$\begin{pmatrix} \tilde{v}_1 \\ \vdots \\ \tilde{v}_N \end{pmatrix} = U^\dagger \cdot \begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix} \qquad ; \qquad \begin{pmatrix} \tilde{A}_{11} & \cdots & \tilde{A}_{1N} \\ \vdots & \ddots & \vdots \\ \tilde{A}_{N1} & \cdots & \tilde{A}_{NN} \end{pmatrix} = U^\dagger \cdot \overbrace{\begin{pmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{N1} & \cdots & A_{NN} \end{pmatrix}}^{\cdot\, U}$$

Exercise 1.3.3

Write a function *basis_change* that receives a change of basis matrix U_{ij} with $|\tilde{e}_j\rangle = \sum_i U_{ij}|e_i\rangle$, the components v_i of a vector, or A_{ij} of an operator, and returns the components $\tilde{v}_i$ or $\tilde{A}_{ij}$ in the new basis.

solution

Exercise 1.3.4

The matrix $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ represents an operator σ_y in the basis $\{|0\rangle, |1\rangle\}$. Write σ_y in the basis $\{|+i\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle), |-i\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)\}$.

solution

1.0.4 Completeness relation

The action of the identity operator is

$$I|v\rangle = |v\rangle$$

In particular, on every basis element $I|i\rangle = |i\rangle$. In other words,
the identity operator I has matrix elements $I_{ij} = \delta_{ij} = \mathrm{diagonal}(1, 1, \ldots, 1)$, so that

$$I = \sum_i |i\rangle\langle i| = \sum_{ij} \delta_{ij} |i\rangle\langle j|$$

This expression is also known as the completeness relation or the closure relation and is used very frequently.

Note: The completeness relation is, in fact, a property of any basis.

In other words, if $\{|e_i\rangle\}$ and $\{|\tilde{e}_i\rangle\}$ are both bases, then $I|e_i\rangle = |e_i\rangle$ and $I|\tilde{e}_j\rangle = |\tilde{e}_j\rangle$, so $+1$ is the only eigenvalue of I in any basis, and the spectral decomposition gives

$$I = \sum_i |e_i\rangle\langle e_i| = \sum_j |\tilde{e}_j\rangle\langle\tilde{e}_j|\,.$$

The closure, or completeness, relation can **always be inserted** at any step of a calculation. It is frequently used to perform changes of basis.

For example, let's see that the inner product $\langle u|v\rangle$ can be calculated in any basis.

Let $|u\rangle = \sum_i u_i|e_i\rangle = \sum_i \tilde{u}_i|\tilde{e}_i\rangle$ and $|v\rangle = \sum_i v_i|e_i\rangle = \sum_i \tilde{v}_i|\tilde{e}_i\rangle$

Then

$$\langle v|u\rangle = \langle v|I|u\rangle = \langle v|\left(\sum_i |e_i\rangle\langle e_i|\right)|u\rangle = \sum_i \langle v|e_i\rangle\langle e_i|u\rangle = \sum_i v_i^* u_i$$

$$\langle v|u\rangle = \langle v|I|u\rangle = \langle v|\left(\sum_i |\tilde{e}_i\rangle\langle\tilde{e}_i|\right)|u\rangle = \sum_i \langle v|\tilde{e}_i\rangle\langle\tilde{e}_i|u\rangle = \sum_i \tilde{v}_i^* \tilde{u}_i$$

2 Lin($\mathcal{H}$) as a vector space

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The set of **all** linear operators over a vector space $\mathcal{H}$ naturally has the structure of a vector space, which we denote by Lin($\mathcal{H}$).

Given two operators, A and B, both the sum $C = A + B$ and the multiplication by a complex number $D = \lambda A$ are *new operators* defined by their action on any vector $|v\rangle \in \mathcal{H}$.

$$C|v\rangle \;=\; (A+B)|v\rangle = A|v\rangle + B|v\rangle$$

$$D|v\rangle \;=\; (\lambda A)|v\rangle = \lambda(A|v\rangle)$$

Adjoint operator

The *adjoint* conjugation can be extended to Lin($\mathcal{H}$)

$$\dagger \;\rightarrow\; \left\{\begin{array}{ccc} z & \leftrightarrow & z^* \\ |u\rangle & \leftrightarrow & \langle u| \\ A & \leftrightarrow & A^\dagger \end{array}\right.$$

and there are two more rules that allow applying † to sums and products of objects $a \in \{z, |u\rangle, A\}$

- *linearity* $(a+b)^\dagger = a^\dagger + b^\dagger$
- *transpose* $(ab)^\dagger = b^\dagger a^\dagger$ (only relevant when a and b do not commute)

Examples 1. \$ |v⟩ = $A|u\rangle$˜˜

Naturally, this equation translates into the same equation for the associated matrices in *any basis*

$$(U_{ij})^\dagger = U_{ji}^* = U_{ij}^{-1}$$

Let us now see why we have defined this class of operators.

Theorem:
The action of a unitary operator preserves the inner product of any two vectors intact.

Proof

Let U be a unitary operator, and $|\varphi'\rangle = U|\varphi\rangle$ and $|\psi'\rangle = U|\psi\rangle$ be two vectors transformed by U, then

$$\langle\varphi'|\psi'\rangle = \Big(\langle\varphi|U^\dagger\Big)\, U|\psi\rangle = \langle\varphi|U^\dagger U|\psi\rangle = \langle\varphi|\psi\rangle$$

Specializing to $|\varphi\rangle = |\psi\rangle$, we have that a unitary operator *preserves the norm.*

$$\|U|\varphi\rangle\| = \||\varphi\rangle\|$$

- In particular, it preserves the norm of any vector.
- Therefore, it preserves the *distance* between two vectors, $d(|v\rangle, |w\rangle) = \||v\rangle - |w\rangle\|$.
- **Composition** of unitary operators **is** unitary

$$(UV)^\dagger = V^\dagger U^\dagger = V^{-1}U^{-1} = (UV)^{-1}$$

Mathematically, this means that unitary operators form a *group.*

- **Linear combination** of unitary operators **is not** unitary

$$(aU + bV)^\dagger = a^*U^\dagger + b^*V^\dagger = a^*U^{-1} + b^*V^{-1} \neq (aU + bV)^{-1}$$

Mathematically, this means that unitary operators **do not form** a *vector subspace* of $\mathrm{Lin}(\mathcal{H})$.

- Therefore, unitary operators do not form a vector subspace within $\mathrm{Lin}(\mathcal{H})$. The mathematical structure they form is called a group: the unitary group $U(d)$ acts on the Hilbert space $\mathcal{H}$ of dimension d.
- Nevertheless, they form a *manifold*: a continuous set that can be parameterized by a collection of parameters, called the *dimension of the manifold.*
- Since there is a one-to-one correspondence between an operator and a matrix (in a basis), that dimension will be equal to the *dimension of the set of unitary matrices.*

Exercise 1.3.4

Subtract from $\dim_{\mathbf{R}}(\mathrm{Lin}(\mathcal{H})) = 2N^2$ the number of equations that restrict the matrix of a unitary operator, and thus find the (real) dimension of the group $U(N)$ of unitary operators of dimension N.

2.0.2 Orthonormal bases

- As a particular case, applying a unitary operator U to an orthonormal basis $\{|e_i\rangle\}$ yields another orthonormal basis $\{|\tilde{e}_i\rangle\}$

$$\left.\begin{array}{c} |\tilde{e}_i\rangle = U|e_i\rangle \\ U^{-1} = U^\dagger \end{array}\right\} \quad \Longleftrightarrow \quad \langle \tilde{e}_i|\tilde{e}_j\rangle = \langle \tilde{e}_i|U^\dagger U|\tilde{e}_j\rangle = \langle e_i|e_j\rangle = \delta_{ij}$$

Conversely, given two orthonormal bases, $\{|e_i\rangle\}$ and $\{|\tilde{e}_i\rangle\}$, the operator relating them is a unitary operator

$$U = \sum_i |\tilde{e}_i\rangle\langle e_i| \quad \Rightarrow \quad U|e_j\rangle = |\tilde{e}_j\rangle$$

$$U^\dagger = \sum_i |e_i\rangle\langle \tilde{e}_i| \quad \Rightarrow \quad U^\dagger|\tilde{e}_j\rangle = |e_j\rangle \quad \Rightarrow \quad U^\dagger = U^{-1}$$

- An orthogonal operator is a particular case of a unitary operator with *real matrix elements*. The rotation operator $R(\theta)$ that we studied at the beginning of this topic is an orthogonal operator. It is straightforward to verify that

$$R(\theta)^\dagger = R(\theta)^t = R(-\theta) = R(\theta)^{-1}$$

[2]:
```
U=np.matrix([[1,1J],[1J, + 1]])/np.sqrt(2)
array_to_latex(U)
```

[2]:

$$\begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}$$

[5]:
```
Uadj=U.getH() # getH es un método de la clase matrix que devuelve la matriz␣
↪conjugada hermítica
array_to_latex(Uadj)
```

[5]:

$$\begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}i}{2} \\ -\frac{\sqrt{2}i}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}$$

[6]:
```
print('check that U is unitary')

array_to_latex(np.dot(Uadj,U))
```

```
check that U is unitary
```

[6]:

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Normal Operator

Definition: An operator N is normal if it commutes with its adjoint

$$NN^\dagger = N^\dagger N$$

The matrix N_{ij} has an important property.

Theorem:
N_{ij} is the matrix of a normal operator, $[N, N^\dagger] = 0$, if and only if it is unitarily equivalent to a diagonal matrix.

That is, if there exists U with $U^{-1} = U^\dagger$ such that

$$N'_{ij} = (U^\dagger N\, U)_{ij} = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_D \end{bmatrix}$$

Hermitian Operator

Definition: An operator H is Hermitian (or self-adjoint) if it satisfies the following equation

$$H = H^\dagger$$

Obviously, a Hermitian operator $\Rightarrow$ is a normal operator, but the converse does not necessarily hold.

- **Linear combination** of *Hermitian* operators with **real** coefficients **is** Hermitian

$$C^\dagger = (aA + bB)^\dagger = a^* A^\dagger + b^* B^\dagger = aA + bB = C$$

Mathematically: the self-adjoint operators form a real vector subspace $\mathrm{Her}(\mathcal{H}) \subset \mathrm{Lin}(\mathcal{H})$.

- **Composition** of Hermitian operators is generally **not** Hermitian

$$(AB)^\dagger = B^\dagger A^\dagger = BA \neq AB$$

Mathematically, they do not form a group unless A and B commute with each other, in which case they form an *Abelian group*.

- The matrix associated with a Hermitian operator is also called Hermitian, and it equals its conjugate transpose.

$$A_{ij} = A^{\dagger}_{ij} \equiv A^{*t}_{ij} = A^{*}_{ji}$$

Note:

From any operator $C \neq C^{\dagger}$, we can always construct a Hermitian operator $H = H^{\dagger}$ by the linear combination

$$H = C + C^{\dagger}$$

where a is a real number. This trivially extends to the matrices representing them in any basis

$$H_{ij} = C_{ij} + C^{*}_{ji}$$

Exercise 1.3.5

Subtract from $\dim_{\mathbf{R}}(\mathrm{L}(\mathcal{H})) = 2N^2$ the number of equations that constrain the matrix of a Hermitian operator and thus find the (real) dimension of the vector subspace of Hermitian operators.

If you have done the last two exercises, you will have found the same answer in both. This means there could be a relationship between Hermitian and unitary matrices.

Positive Semidefinite Operator

Definition: we say that an operator A is positive semidefinite (or non-negative) if it satisfies

$$\langle u|A|u\rangle \geq 0$$

for all $|u\rangle \in \mathcal{H}$.

In this case, we write $A \geq 0$.

If the inequality is strict, $\langle u|A|u\rangle > 0$ for all $|u\rangle$, then A is called a *positive operator*, denoted $A > 0$.

The following theorem is the equivalent of the fact that a real number $a \in \mathbb{R}$ has a square root if and only if it is non-negative.

Theorem: A Hermitian operator A is positive semidefinite if and only if there exists another operator B such that

$$A = B^{\dagger}B$$

for all $|u\rangle \in \mathcal{H}$.

Projectors

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Definition:
A projector is a Hermitian operator that satisfies the equation

$$P^2 = P$$

- The operator $P = |u\rangle\langle u|$ fulfills it is Hermitian

$$P^\dagger = |u\rangle\langle u| = P$$

- it is idempotent

$$P^2 = |u\rangle\langle u|u\rangle\langle u| = |u\rangle\langle u| = P$$

- It indeed projects **any vector** onto the direction of $|u\rangle$

$$P|w\rangle = |u\rangle\langle u|w\rangle = a|u\rangle$$

where the complex number $a = \langle u|w\rangle$ is the **projection**

Note:

- The projection is non-invertible
- The projector is a non-unitary operator: in general it reduces the norm

  $$\|P|w\rangle\|^2 = \langle w|P^\dagger P|w\rangle = \langle w|P|w\rangle = \langle w|u\rangle\langle u|w\rangle = |\langle u|w\rangle|^2 < \||u\rangle\|\||w\rangle\| = 1$$

  where we have applied the Cauchy-Schwarz inequality, which is strict if we assume $|u\rangle \neq |w\rangle$.
-

2.0.3 Matrix associated to a projector

If $|u\rangle = |e_1\rangle$, the operator $P_1 = |e_1\rangle\langle e_1|$ projects any vector onto its component along $|e_1\rangle$.

In matrix form

$$|e_1\rangle\langle e_1| = \begin{pmatrix} 1 & 0 & ... & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

so that

$$|e_1\rangle\langle e_1|u\rangle \;=\; \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix} = \begin{pmatrix} u^1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = u^1|e_1\rangle$$

If $|u\rangle = \sum_i u^i|e_i\rangle$ is a unit vector with $\||u\rangle\| = 1$, then the projector along $|u\rangle$ is given by

$$P(u) = |u\rangle\langle u| = \sum_{i,j} u_i u_j^* |e_i\rangle\langle e_j|$$

That is, it is associated with a matrix given by $P_{ij} = u_i u_j^*$. It is straightforward to verify that

$$P_{ik}^2 = \sum_j P_{ij} P_{jk} = \sum_j u_i u_j^* u_j u_k^* = u_i \left(\sum_j u_j^* u_j \right) u_k^* = u_i u_k^* = P_{ik}$$

as corresponds to a projector.

Orthogonal projectors

- P_1 and P_2 are orthogonal projectors if they satisfy

$$P_1^2 = P_1 \qquad P_2^2 = P_2 \qquad P_1 P_2 = P_2 P_1 = 0$$

- if P_1 and P_2 are orthogonal projectors, $P = P_1 + P_2$ is also a projector

$$P^2 = (P_1 + P_2)(P_1 + P_2) = P_1^2 + P_1 P_2 + P_2 P_1 + P_2^2 = P_1 + P_2 = P$$

- A particularly important case of orthogonal proyectors is $P_1 = P$ and $P_2 = P_\perp = I - P$.

    Proof

indeed $P_\perp$ is a projector

$$P_\perp^2 = (I - P)(I - P) = I^2 - P - P + P^2 = I - P = P_\perp$$

and it is perpendicular to P

$$P_\perp P \;\; = \;\; (I - P)P = P - P^2 = P - P = 0 \tag{11}$$

Given a vector $|u\rangle$, we can decompose any other vector $|\psi\rangle$ into its parallel and perpendicular projections

$$|\psi\rangle = (P + P_\perp)|\psi\rangle = a|u\rangle + b|u_\perp\rangle$$

where $a = \langle u|\psi\rangle$ and $b = \langle u_\perp|\psi\rangle$

The equation $|\psi\rangle = a|u\rangle + b|u_\perp\rangle$ means that the three vectors lie in the same hyperplane.

[3]:
```
d = 3

' generate a random vector'
u = tQ.random_ket(d)
display(array_to_latex(u))

' build the parallel and perpendicular projectors'
P_par = tQ.ket_bra(u,u);
P_perp = np.identity(d) - P_par
```

```
display(array_to_latex(P_par))
display(array_to_latex(P_perp))
```

$$\begin{bmatrix} -0.6097923742 - 0.454015077i \\ 0.1887022679 - 0.2144934205i \\ -0.4145697439 + 0.4105356555i \end{bmatrix}$$

$$\begin{bmatrix} 0.5779764297 & -0.0176859571 - 0.2164701268i & 0.0664120911 + 0.4385624262i \\ -0.0176859571 + 0.2164701268i & 0.0816159733 & -0.1662874478 + 0.0114534731i \\ 0.0664120911 - 0.4385624262i & -0.1662874478 - 0.0114534731i & 0.3404075969 \end{bmatrix}$$

$$\begin{bmatrix} 0.4220235703 & 0.0176859571 + 0.2164701268i & -0.0664120911 - 0.4385624262i \\ 0.0176859571 - 0.2164701268i & 0.9183840267 & 0.1662874478 - 0.0114534731i \\ -0.0664120911 + 0.4385624262i & 0.1662874478 + 0.0114534731i & 0.6595924031 \end{bmatrix}$$

[7]:

```
' check properties P^2 = P, and orthogonality '
A = P_par@P_par - P_par
B = P_perp@P_perp - P_perp
C = P_par@P_perp

display(array_to_latex(C))


' obtain parallel and perpendicular components of another vector'
v = tQ.random_ket(d)

v_par = np.dot(P_par,v)
v_perp = np.dot(P_perp,v)

' check perpendicularity'
print(np.round(tQ.braket(v_par,v_perp),4))
```

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

0j

Exercise 1.3.6 (reflector)

Given a unit vector $(|\mathrm{u}\rangle), writedown:$

- the operator (R_u^{$\perp$})$thatreflectsthecomponentperpendicularto(|u\rangle)ofanyvector(|\psi\rangle)$

- the operator (R_u^{|}) that reflects the component parallel to $(|\mathrm{u}\rangle)ofanyvector(|\psi\rangle)$

2.0.4 Projectors onto a Subspace

Consider an orthonormal basis $\{|e_i\rangle\}, i = 1, \ldots, N$ of $\mathcal{H}$, and divide it into two subsets

$$\{|e_i\rangle\}, \quad i = 1, \ldots, N_1 \quad , \quad \{|e_{j+N_1}\rangle\}, \quad j = 1, \ldots, N_2$$

Any vector admits an orthogonal decomposition

$$|\psi\rangle \quad = \quad \sum_{i=1}^{N} a_i |e_i\rangle = \sum_{i=1}^{N_1} a_i |e_i\rangle + \sum_{i=1}^{N_2} a_{i+N_1} |e_{i+N_1}\rangle \equiv |\psi_1\rangle + |\psi_2\rangle \quad (12)$$

(12)

with $\langle\psi_1|\psi_2\rangle = 0$.

We say that the space H decomposes into the *direct sum of orthogonal subspaces*

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$$

of dimensions $N_1 + N_2 = N$,

The operators

$$P_1 = \sum_{i=1}^{N_1} |e_i\rangle\langle e_i| \quad , \quad P_2 = \sum_{i=1}^{N_2} |e_{i+N_1}\rangle\langle e_{i+N_1}| = I - P_1$$

are orthogonal projectors projector

$$P_1^2 = P_1 \quad , \quad P_2^2 = P_2 \quad , \quad P_1 P_2 = P_2 P_1 = 0$$

Their action extracts from a vector its component in the associated subspace.

$$P_1|\psi\rangle \;=\; \sum_{i=1}^{N_1} |e_i\rangle\langle e_i| \left(\sum_{k=1}^{N} a_k|u_k\rangle\right) \;=\; \sum_{i=1}^{N_1} a_i|e_i\rangle \;=\; |\psi_1\rangle$$

$$P_2|\psi\rangle \;=\; \sum_{i=1}^{N_2} |e_{i+N_1}\rangle\langle e_{i+N_1}| \left(\sum_{k=1}^{N} a_k|u_k\rangle\right) \;=\; \sum_{i=1}^{N_1} a_{i+N_1}|e_{i+N_1}\rangle \;=\; |\psi_2\rangle$$

Note:

$P_1 \neq P_v = |v\rangle\langle v|$ where $|v\rangle = \sum_i |i\rangle$. This operator would project any vector onto the direction of $|v\rangle$.

Eigenvalues and eigenvectors

«<

Definition: Eigenvalues and eigenvectors There exist vectors, $|\lambda\rangle$, for which the action of an operator A returns a parallel vector

$$A|\lambda\rangle = \lambda|\lambda\rangle$$

We say that $|\lambda\rangle$ is an eigenvector (or proper vector) of A with associated eigenvalue (or proper value) $\lambda \in \mathbb{C}$

Suppose that A has d eigenvectors $|\lambda_j\rangle = \sum_i v_{ij}|e_i\rangle$, $j = 1, \ldots, d$.

Let $U_{ij} = v_{ij}$ be the matrix formed by the components of the eigenvectors (stacked as columns).

Then

$$A_{diag} = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_d \end{pmatrix} = U^{-1}AU$$

If A is normal, the matrix U that diagonalizes it is unitary, i.e., $U^{-1} = U^\dagger$.

[7]:
```
d = 2
' en general una matriz no será normal '
A = np.matrix(np.random.rand(d,d)+ np.random.rand(d,d) * 1j)
display(array_to_latex(np.dot(A,A.getH()) - np.dot(A.getH(),A)))

eigvals, eigvecs = np.linalg.eig(A)
print('valprop =',eigvals)

'verificamos que los autovectores son las columnas de v'
m=1 #cambiar a otro valor
display(array_to_latex(np.dot(A, eigvecs[:, m]) - eigvals[m] * eigvecs[:,␣
↪m],prefix=r'A|\lambda_m \rangle -\lambda_m |\lambda_m\rangle =  '))

' diagonalizamos A '
U = np.matrix(eigvecs);
```

```
array_to_latex(np.dot(U.getI(),np.dot(A,U)),prefix='A_{diag} = U^{-1} A U = ')

'U no es unitaria'
array_to_latex(np.dot(U,U.getH()))
```

$$\begin{bmatrix} 0.0362223694 & -0.147799331+0.6577739833i \\ -0.147799331-0.6577739833i & -0.0362223694 \end{bmatrix}$$

```
valprop = [0.34791292-0.50406172j 1.05867426+1.35722234j]
```

$$A|\lambda_m\rangle - \lambda_m|\lambda_m\rangle = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

[7]:

$$\begin{bmatrix} 1.0088753185 & -0.0362142552+0.1611698425i \\ -0.0362142552-0.1611698425i & 0.9911246815 \end{bmatrix}$$

[8]:
```
d = 2
'veamos ahora una matriz normal'
A = np.matrix([[1, -1], [1, 1]])
display(array_to_latex(np.dot(A,A.getH()) - np.dot(A.getH(),A)))


eigvals, eigvecs = np.linalg.eig(A)
print('valprop =',eigvals)

'verificamos que los autovectores son las columnas de v'
m=1 #cambiar a otro valor
display(array_to_latex(np.dot(A, eigvecs[:, m]) - eigvals[m] * eigvecs[:,␣
 ↪m],prefix=r'A|\lambda_m \rangle -\lambda_m |\lambda_m\rangle =  '))

' diagonalizamos A '
U = np.matrix(eigvecs);

array_to_latex(np.dot(U.getH(),np.dot(A,U)),prefix='A_{diag} = U^{\dagger} A U =␣
 ↪')

'U es unitaria'
array_to_latex(np.dot(U,U.getH()))
```

$$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

```
valprop = [1.+1.j 1.-1.j]
```

$$A|\lambda_m\rangle - \lambda_m|\lambda_m\rangle = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

[8]:

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Eigenspaces

«<

We say that an eigenvalue λ_k is d_k-fold *degenerate* if there exist d_k linearly independent eigenvectors, $|\lambda_k^a\rangle$ with $a = 1, ..., d_k$, associated to the **same** eigenvalue

$$A|\lambda_k^a\rangle = \lambda_k|\lambda_k^a\rangle$$

These eigenvectors generate an *eigenspace* $S(\lambda_k) \subset \mathcal{H}$.

For example, let $|u\rangle = \sum_{a=1}^{d_k} c_a|\lambda_k^a\rangle$ be a linear combination of these eigenvectors, then

$$A|u\rangle = \sum_{a=1}^{d_k} c_a A|\lambda_k^a\rangle = \sum_{a=1}^{d_k} c_a\lambda_k|\lambda_k^a\rangle = \lambda_k \sum_{a=1}^{d_k} c_a|\lambda_k^a\rangle = \lambda_k|u\rangle \tag{13}$$

Therefore, $|u\rangle \in S(\lambda_k)$.

- The Gram-Schmidt theorem guarantees that we can choose (through an appropriate change) the set $\{|\lambda_k^a\rangle\} \in (\lambda_k), a = 1, \ldots, d_k$ so that it forms an orthonormal basis

$$\langle\lambda_k^a|\lambda_k^b\rangle = \delta_{ab}$$

- The **orthogonal projector** onto the eigenspace $S(\lambda_k)$ is

$$P_k = \sum_{a=1}^{d_k} |\lambda_k^a\rangle\langle\lambda_k^a|$$

Example:

- Let us denote by $R_z(\theta)$ the operator that performs a rotation in the (x, y) plane by an angle θ. When $\theta = \pi$ we have the following action on the three elements $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}\}$ of the Cartesian basis:

$$R_z(\pi)\hat{\mathbf{x}} = -\hat{\mathbf{x}} \tag{14}$$

$$R_z(\pi)\hat{\mathbf{y}} = -\hat{\mathbf{y}} \tag{15}$$

$$R_z(\pi)\hat{\mathbf{z}} = +\hat{\mathbf{z}} \tag{16}$$

- We see that there is an eigenvector $\hat{\mathbf{z}}$ with eigenvalue $+1$ and two eigenvectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ with eigenvalue -1.
- The space $\mathbb{R}^3$ splits into two eigenspaces of $R_z(\pi)$: one of dimension 1 (along the $\hat{\mathbf{z}}$ axis) and another of dimension 2 (in the $(\hat{\mathbf{x}}, \hat{\mathbf{y}})$ plane).

- The associated projectors are

$$P_{\hat{\mathbf{z}}} = |\hat{\mathbf{z}}\rangle\langle\hat{\mathbf{z}}| = \begin{bmatrix} 0 & & \\ & 0 & \\ & & 1 \end{bmatrix} \quad , \quad P_{\hat{\mathbf{x}}\hat{\mathbf{y}}} = |\hat{\mathbf{x}}\rangle\langle\hat{\mathbf{x}}| + |\hat{\mathbf{y}}\rangle\langle\hat{\mathbf{y}}| = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 0 \end{bmatrix} \quad ,$$

2.1 Operators' spectra

2.1.1 Spectrum of Normal Operators

Let us recall that N is a normal operator if it commutes with its adjoint:

$$NN^\dagger = N^\dagger N$$

Spectra of normal operators enjoy an important property

Theorem: the eigenvectors of a normal operator associated to two distinct eigenvalues are orthogonal

$$\lambda_i \neq \lambda_j \qquad \Longleftrightarrow \qquad \langle\lambda_i|\lambda_j\rangle = 0$$

Proof:

From the eigenvalue equation $N|\lambda_j\rangle = \lambda_j|\lambda_j\rangle$ and from $NN^\dagger = N^\dagger N$, it follows that

$$\langle\lambda_j|(N^\dagger - \lambda_j^*)(N - \lambda_j)|\lambda_j\rangle = \langle\lambda_j|(N - \lambda_j)(N^\dagger - \lambda_j^*)|\lambda_j\rangle = 0\,,$$

from which we obtain $(N^\dagger - \lambda_j^*)|\lambda_j\rangle = 0 \Rightarrow \langle\lambda_j|N = \langle\lambda_j|\lambda_j$. Then

$$\langle\lambda_j|N|\lambda_i\rangle = \lambda_j\langle\lambda_j|\lambda_i\rangle = \lambda_i\langle\lambda_j|\lambda_i\rangle\,,$$

from which it follows that, for $\lambda_i \neq \lambda_j$, $\Rightarrow \langle\lambda_i|\lambda_j\rangle = 0$.

In general, each eigenvalue λ_k will be degenerate $d_k \geq 1$ times.

In that case, there are $\{|\lambda_k^a\rangle\}, a = 1, ..., d_k$ eigenvectors that generate the eigenspace, $S(\lambda_k) \subset \mathcal{H}$, of dimension d_k.

Subspaces $S(\lambda_k) \perp S(\lambda_j)$ are orthogonal for $k \neq j$ according to the lemma.

In summary: we can always find an orthonormal basis of $\mathcal{H}$, formed by eigenvectors of a normal operator N

$$I = \sum_k \sum_{a=1}^{d_k} |\lambda_k^a\rangle\langle\lambda_k^a| \quad ; \quad \langle\lambda_j^a|\lambda_k^b\rangle = \delta_{ab}\delta_{jk}$$

The projector onto the eigenspace $S(\lambda_k)$ is

$$P_k = \sum_{a=1}^{d_k} |\lambda_k^a\rangle\langle\lambda_k^a|$$

2.1.2 Spectrum of Hermitian Operators

The spectrum of a Hermitian operator $A = A^\dagger$ has two important properties:
- 1. The eigenvalues of a Hermitian operator are real $\lambda_i \in \mathbb{R}$.
- 2. The eigenvectors $|\lambda_i\rangle$ of a Hermitian operator associated with distinct eigenvalues are orthogonal

$$\lambda_i \neq \lambda_j \quad \Longleftrightarrow \quad \langle\lambda_i|\lambda_j\rangle = 0 \,.$$

Proof:

1. Take a normalized eigenvector of A, $|\lambda\rangle$ with eigenvalue λ.

$$\lambda = \langle\lambda|A|\lambda\rangle = (\langle\lambda|A^\dagger|\lambda\rangle)^* = (\langle\lambda|A|\lambda\rangle)^* = \lambda^*.$$

2. In fact, this property holds for normal operators N. Hermitian operators are normal. From the eigenvalue equation $N|\lambda_j\rangle = \lambda_j|\lambda_j\rangle$ and $NN^\dagger = N^\dagger N$, it follows that

$$\langle\lambda_j|(N^\dagger - \lambda_j^*)(N - \lambda_j)|\lambda_j\rangle = \langle\lambda_j|(N - \lambda_j)(N^\dagger - \lambda_j^*)|\lambda_j\rangle = 0 \,,$$

from which we get $(N^\dagger - \lambda_j^*)|\lambda_j\rangle = 0 \Rightarrow \langle\lambda_j|N = \langle\lambda_j|\lambda_j$. Then

$$\langle\lambda_j|N|\lambda_i\rangle = \lambda_j\langle\lambda_j|\lambda_i\rangle = \lambda_i\langle\lambda_j|\lambda_i\rangle \,,$$

from which it follows that for $\lambda_i \neq \lambda_j \Rightarrow \langle\lambda_i|\lambda_j\rangle = 0$.

The set of eigenvectors $|\lambda_i\rangle$ of a Hermitian operator forms an orthogonal basis. It can be normalized to form an orthonormal basis

$$\langle\lambda_i|\lambda_j\rangle = \delta_{ij}$$

Exercise 1.3.7

Write a function, *random_hermitian*, that generates a Hermitian matrix of dimension d.
Verify in different cases that the spectrum is real.

2.1.3 Spectrum of Unitary Operators

The eigenvalues of a unitary operator are pure phases

$$U^\dagger = U^{-1} \quad \iff \quad \lambda_i = e^{i\phi_i}$$

Proof

Your proof here

2.1.4 Spectrum of Proyectors

Prueba

La ecuación

$$P^2 = P \qquad \Rightarrow \qquad P^2|u\rangle = P|u\rangle$$

sólo tiene dos soluciones consistentes

$$P|u\rangle = |u\rangle \qquad \text{y} \qquad P|u\rangle = 0$$

2.1.5 Commuting Operators

When two operators commute, certain algebraic properties arise that are very advantageous. In a way, they behave more like c-numbers. Let's see the first one.

Theorem
Given two operators A and B that commute, there exists a basis $\{|\lambda_i\rangle\}$ of simultaneous eigenvectors of both operators, that is

$$A = \lambda_i^A |\lambda_i\rangle\langle\lambda_i| \quad , \qquad B = \lambda_i^B |\lambda_i\rangle\langle\lambda_i|$$

Proof

Suppose A and B commute. Then the action of A *stabilizes* the eigenspaces of B.

That is, if $|\lambda\rangle$ is an eigenstate of B, then $B|\lambda\rangle = |\mu\rangle$ is also an eigenstate with the same eigenvalue. It is straightforward to verify:

$$A(B|\lambda\rangle) = B(A|\lambda\rangle) = B(\lambda|\lambda\rangle) = \lambda(B|\lambda\rangle)$$

Therefore, $|\lambda\rangle$ and $B|\lambda\rangle$ belong to the *same eigenspace*. This is what is meant by *stabilizing the subspace.*

If λ is degenerate, this only ensures that $B|\lambda\rangle = |\lambda'\rangle$ belongs to the eigenspace of the same eigenvalue λ.

This means that within each eigenspace of B, we can choose any basis we want. In particular, we can choose a basis that diagonalizes A within that subspace.

In other words, two operators that commute are simultaneously diagonalizable. Their matrices in the basis $\{|\lambda_i\rangle\}$ are

$$A = \begin{bmatrix} \lambda_1^A & 0 & \cdots & 0 \\ 0 & \lambda_2^A & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^A \end{bmatrix}, \quad B = \begin{bmatrix} \lambda_1^B & 0 & \cdots & 0 \\ 0 & \lambda_2^B & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^B \end{bmatrix}$$

2.1.6 Singular Values

Let $A \in \text{Lin}(\mathcal{H})$ be a general operator. Then $A^\dagger A$ is a Hermitian operator that has non-negative eigenvalues $\lambda_i \geq 0$

$$A^\dagger A|\lambda_i\rangle = \lambda_i|\lambda_i\rangle \quad \Rightarrow \quad \lambda_i = \langle\lambda_i|A^\dagger A|\lambda_i\rangle = \|A|\lambda_i\rangle\|^2 \geq 0$$

Therefore, we can take its square root $s_i = \sqrt{\lambda_i} \geq 0$.

Definition: The singular values of $A \in \text{Lin}(\mathcal{H})$ are defined as $s_i = \sqrt{\lambda_i}$ where λ_i are the eigenvalues of the operator $A^\dagger A$.

Singular values are very important to characterize the difference between two operators, as we will see later.

Operator decompositions «<

Spectral decomposition

Theorem: Spectral Decomposition

For every normal operator N there exists a basis of orthonormal eigenvectors, $\{|\lambda_k^a\rangle\}$, such that N admits the following spectral decomposition

$$N = \sum_{k=1}^{d} \lambda_k P_k \,.$$

Here $d = \dim(\mathcal{H})$ and $P_k = \sum_{a=1}^{g_k} |\lambda_k^a\rangle\langle\lambda_k^a|$ is the projector onto the eigenspace $S(\lambda_k)$, where λ_k is g_k-fold degenerate.

[2]:
```
A = np.array([[1, 1], [-1, 1]])
array_to_latex(A, prefix = 'A = ')
```

[2]:

$$A = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$$

[4]:
```
' Realizamos la descomposición espectral'
eigvals, eigvecs = np.linalg.eig(A)

eigvec0 = eigvecs[:,0]
P0 = tQ.ket_bra(eigvec0,eigvec0)
display(array_to_latex(P0,prefix='P_0='))
```

```python
eigvec1 = eigvecs[:,1]
P1 = tQ.ket_bra(eigvec1,eigvec1)
display(array_to_latex(P1,prefix='P_1='))

'verificamos completitud'
array_to_latex(P0+P1,prefix='P_0 + P_1=')
```

$$P_0 = \begin{bmatrix} \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & \frac{1}{2} \end{bmatrix}$$

$$P_1 = \begin{bmatrix} \frac{1}{2} & \frac{i}{2} \\ -\frac{i}{2} & \frac{1}{2} \end{bmatrix}$$

[4]:

$$P_0 + P_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

[6]:

```python
A_descomp_espect = eigvals[0]*P0+eigvals[1]*P1

array_to_latex(A_descomp_espect, prefix = '\lambda_ 0 P_0 + \lambda_1 P_1 =  ')
```

[6]:

$$\lambda_0 P_0 + \lambda_1 P_1 = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$$

The matrix A_{ij} that represents A in the basis $|\lambda_i\rangle$ is diagonal

$$A_{ij} = \langle \lambda_i^a | A | \lambda_j^b \rangle = \lambda_k \delta_{kj} \delta_{ab} = \begin{bmatrix} \lambda_1 & & & & \\ & \ddots & & & \\ & & \lambda_2 & & \\ & & & \ddots & \\ & & & & \lambda_N \end{bmatrix}$$

where λ_k appears repeated d_k times.

Note:

The identity operator has every vector as an eigenvector $I|v\rangle = |v\rangle$, with eigenvalues $\lambda_i = 1$. Therefore, in any basis, the matrix associated to I has diagonal form

$$I_{ij} = \delta_{ij} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}$$

The spectral decomposition of I is none other than the completeness relation, which holds *for any basis*, since all bases are eigenbases of I

$$I \;=\; \sum_{i=1}^{N} |\lambda_i\rangle\langle\lambda_i| \;=\; \sum_{i=1}^{N} |e_i\rangle\langle e_i|$$

Exercise 1.3.8

Write a Python function *spectral_decomp* that returns the two lists λ_i and P_i associated with the spectral decomposition of a diagonalizable operator $A = \sum_i \lambda_i P_i$.

Suppose we only know the spectrum of eigenvalues $\{\lambda_i\}$ of A and not its eigenvectors. Even so, the projector P_i can be written as

$$P_i = \prod_{k\neq i} \frac{A - \lambda_k I}{\lambda_i - \lambda_k}$$

By construction, it holds that

$$P_i|\lambda_j\rangle = \delta_{ij}|\lambda_j\rangle \quad , \quad AP_i = \lambda_i P_i\,.$$

Note that the range of P_i is included by construction without needing to know the basis generating the subspace $\{|\lambda_{i,p}\rangle\}$.

Spectral Representation of Projectors

Let A be a normal matrix with eigenvalues λ_i and eigenvectors $|\lambda_{i,p}\rangle, p = 1, ..., g_i = \deg(\lambda_i)$,

$$P_i = \sum_{p=1}^{g_i} |\lambda_{i,p}\rangle\langle\lambda_{i,p}|$$

is a projector onto the eigenspace associated with λ_i.

Polar Decomposition (PD)

Theorem:
Every operator $A \in \mathrm{Lin}(\mathcal{H})$ admits a polar decomposition $A = UR$ where U is a unitary operator, and R is a positive semi-definite operator (having only non-negative eigenvalues).

- The polar decomposition is *unique* and generalizes the polar representation of complex numbers $z = re^{i\phi}$ to operators.

- The fact that $r \geq 0$ corresponds to R being positive semi-definite.

- The factor $e^{i\phi}$ is analogous to the fact that a unitary operator, as we will see, has eigenvalues that are pure phases.

Exercise 1.3.9

Write a function *random_unitary* that generates a unitary matrix of dimension d.
Check in various cases that its spectrum consists of phases.

[19]:
```
'''Método para construir una matriz unitaria arbitraria usando la descomposición␣
↪polar'''
d = 3
A = np.matrix(np.random.rand(d,d)+ np.random.rand(d,d) * 1j)

#u, s, vh = linalg.svd(A, full_matrices=False)
```

```
u,r = la.polar(A)

R = np.matrix(r)
' verificamos que R sólo tiene autovalores no-negativos '
Reigval, Reigvec = la.eig(R)
print(np.round(Reigval,3))

U=np.matrix(u)
display(array_to_latex(U, prefix= 'U = '))

''' Verifiquemos unitariedad '''
display(array_to_latex(np.dot(U.getH(),U),prefix='U^{\dagger}U = '))

''' verificamos que los autovalores de U son fases'''
np.round([la.eig(U)[0][i]*la.eig(U)[0][i].conjugate() for i in range(d)],5)
```

```
[2.431+0.j 0.08 +0.j 0.686+0.j]
```

$$U = \begin{bmatrix} 0.6448584703 - 0.0545397974i & 0.27980105 + 0.6601651084i & 0.2589661709 - 0.0035900099i \\ 0.3682011215 + 0.3892475176i & 0.4452677423 - 0.3869059114i & -0.322586681 + 0.5107764587i \\ -0.4459615381 + 0.30857021i & 0.3705983147 + 0.0243052369i & 0.7163582861 + 0.2340933202i \end{bmatrix}$$

$$U^{\dagger}U = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

[19]:
```
array([1.-0.j, 1.+0.j, 1.-0.j])
```

2.1.7 Singular Value Decomposition (SVD)

Singular Value Decomposition Theorem: SVD

Let A be a complex $m \times n$ matrix. Then it admits the following form (singular value decomposition)

$$A = U\,\Sigma\,V^{\dagger}\,,$$

where $U \in U(m)$, $V \in U(n)$ are square unitary matrices and Σ is a rectangular $m \times n$ matrix with the nonzero singular values $s_1, ..., s_r$ of A on the diagonal, where $r \leq \min(m, n)$.

Proof:

Notice that A is the matrix of a linear map $\mathcal{H}_n \to \mathcal{H}_m$, i.e. if $|u\rangle \in \mathcal{H}_n$ then $|v\rangle = A|u\rangle \in \mathcal{H}_m$.

Of utmost importance will be the linear endomorphisms $A^{\dagger}A \in \mathrm{Lin}(\mathcal{H}_n)$ and $AA^{\dagger} \in \mathrm{Lin}(\mathcal{H}_m)$.

Let us start buy showing two things

- they have the same eigenvalues. Indeed, if $|u\rangle \in \mathcal{H}_n$ is eigenvector of $A^\dagger A$ then $|v\rangle = A|v\rangle \in \mathcal{H}_m$ is an eigenvector of $AA^\dagger$ with the same eigenvalue.

$$AA^\dagger|v\rangle = AA^\dagger(A|u\rangle) = A(A^\dagger A|u\rangle) = A\lambda|u\rangle = \lambda A|u\rangle = \lambda|v\rangle$$

- the eigenvalues are real an non-negative. Reality comes out from the hermiticity of $A^\dagger A \in \mathrm{Lin}(H_n)$. Now

$$\lambda_i = \langle\lambda_i|A^\dagger A|\lambda_i\rangle = \|A|\lambda_i\rangle\|^2 \geq 0.$$

Ordered in decreasing order, there are r nonzero eigenvalues, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > 0$.
Their square roots $\sqrt{\lambda_1} \geq \sqrt{\lambda_2} \geq \cdots \geq \sqrt{\lambda_r} > 0$ define the so-called singular values $s_i = \sqrt{\lambda_i}$ of the operator A.

Start by diagonalizing $A^\dagger A$, and obtain an orthonormal basis $|\lambda_i\rangle$. Taking these as column vectors, we can form the following matrices

$$V(n\times n) = \Big(|\lambda_1\rangle, |\lambda_2\rangle, ..., |\lambda_r\rangle, |\lambda_{r+1}\rangle, ..., |\lambda_n\rangle\Big)$$

$$\Sigma(m\times n) = \left.\overbrace{\begin{pmatrix} \sqrt{\lambda_1} & \cdots & & & 0 \\ \vdots & \ddots & & & \vdots \\ & & \sqrt{\lambda_r} & & \\ & & & 0 & \\ & & & & \ddots \\ 0 & & \cdots & & 0 \\ \vdots & & & & \vdots \\ 0 & & \cdots & & 0 \end{pmatrix}}^{n}\right\} m$$

$$U(m\times m) = \left(\frac{1}{\sqrt{\lambda_1}}A|\lambda_1\rangle, \frac{1}{\sqrt{\lambda_2}}A|\lambda_2\rangle, ..., \frac{1}{\sqrt{\lambda_r}}A|\lambda_r\rangle, |\mu_{r+1}\rangle, ...|\mu_m\rangle\right).$$

where $|\mu_{r+1}\rangle, \ldots, |\mu_m\rangle$ complete the orthonormal basis of vectors.

Now we can operate

$$
\begin{aligned}
U\Sigma V^\dagger &= \left(\frac{1}{\sqrt{\lambda_1}}A|\lambda_1\rangle, \frac{1}{\sqrt{\lambda_2}}A|\lambda_2\rangle, ..., \frac{1}{\sqrt{\lambda_r}}A|\lambda_r\rangle, |\mu_{r+1}\rangle, ...|\mu_m\rangle\right)\begin{pmatrix} \sqrt{\lambda_1}\langle\lambda_1| \\ \sqrt{\lambda_2}\langle\lambda_2| \\ \vdots \\ \sqrt{\lambda_r}\langle\lambda_r| \\ 0 \\ \vdots \\ 0 \end{pmatrix} \\
&= A\sum_{i=1}^{r}|\lambda_i\rangle\langle\lambda_i| = A\sum_{i=1}^{n}|\lambda_i\rangle\langle\lambda_i| = A\,,
\end{aligned}
$$

were we used that $A|\lambda_i\rangle = 0$ for $i > r$. This completes the proof. Let us however gain some insight into the nature of matrices U and V.

The following equations hold

$$
A^\dagger A = V\,\Sigma^\dagger U\,U^\dagger \Sigma\,V^\dagger = V\,(\Sigma^\dagger\Sigma)\,V^\dagger \tag{17}
$$

$$
AA^\dagger = U\,\Sigma V^\dagger V\,\Sigma^\dagger U^\dagger = U\,(\Sigma\Sigma^\dagger)\,U^\dagger \tag{18}
$$

or equivalently

$$
\Sigma^\dagger\Sigma = V^\dagger A^\dagger A V \quad , \quad \Sigma\Sigma^\dagger = U^\dagger A A^\dagger U
$$

The matrices

$$
\Sigma\Sigma^\dagger = \mathrm{diag}(\lambda_1, \dots, \lambda_r, 0, \dots, 0)_{m\times m} \quad , \quad \Sigma^\dagger\Sigma = \mathrm{diag}(\lambda_1, \dots, \lambda_r, 0, \dots, 0)_{n\times n}
$$

are diagonal. Therefore:

- The matrix V diagonalizes $A^\dagger A$. Hence its columns are the n eigenvectors of $A^\dagger A$.
- The matrix U diagonalizes $AA^\dagger$. Hence its columns are the m eigenvectors of $AA^\dagger$.

This looks like an efficient way to find the matrices U and V. However this is true only up to diagonal unitaries

Notice that any $\tilde{V} = VD$ and $\tilde{U} = UF$ such that

$$
D^\dagger\Sigma^\dagger\Sigma D = \Sigma^\dagger\Sigma \quad , \quad F^\dagger\Sigma\Sigma^\dagger F = \Sigma\Sigma^\dagger
$$

will lead to a different equivalently valid solution of the form

$$
\Sigma^\dagger\Sigma = \tilde{V}^\dagger A^\dagger A\tilde{V} \quad , \quad \Sigma\Sigma^\dagger = \tilde{U}^\dagger AA^\dagger\tilde{U}
$$

Now

$$\tilde{A} = \tilde{U}\Sigma\tilde{V}^{\dagger} = UD\Sigma F^{\dagger}V^{\dagger} \neq U\Sigma V^{\dagger} = A$$

So, not any element in the equivalence class gives the SVD of A

Note that the rank of U and V is $r \leq m \leq n$. Therefore, there is an ambiguity in the choice of eigenvectors of U and V associated with the zero singular values.

Let's state this theorem for matrices. Specifically, the theorem refers to an $m \times n$ matrix. This type of matrix corresponds to operators $O \in \text{Lin}(\mathcal{H}_A, \mathcal{H}_B)$ between spaces of dimensions m and n.

[7]:
```
'NumPy has the `svd` function to perform singular value decomposition.'
m=3
n=2

A = np.matrix(np.random.randn(m,n)+ 1j*np.random.randn(m,n))
display(array_to_latex(A,prefix='A='))
print( 'the shape of A is :', A.shape)


u, s, vh = la.svd(A, full_matrices=True)


print( 'the shape of u =',u.shape, ' s =', s.shape,' v =', vh.shape)
```

$$A = \begin{bmatrix} -0.5236930728 + 1.9118334053i & 0.5767927192 - 2.0843848053i \\ -0.3643731504 - 1.0819914804i & 0.7246113054 - 0.5586193168i \\ -0.9682747944 - 1.672583164i & -0.9877737104 + 0.3425877513i \end{bmatrix}$$

```
the shape of A is : (3, 2)
the shape of u = (3, 3)  s = (2,)  v = (2, 2)
```

[9]:
```
U=np.matrix(u)
S= np.zeros((m, n))
np.fill_diagonal(S,s)
S = np.matrix(S)
V=np.matrix(vh).getH()

display(array_to_latex(U,prefix='U='))
display(array_to_latex(S,prefix='S='))
display(array_to_latex(V,prefix='V='))

display(array_to_latex(np.round(S@S.getH(),8),prefix='S S^{\dagger} ='))

#'''Verifiquemos unitariedad'''
#display(array_to_latex(np.dot(V.getH(),V),prefix='V^{\dagger}V ='))
#display(array_to_latex(np.dot(U.getH(),U),prefix='U^{\dagger}U ='))
```

$$U = \begin{bmatrix} -0.1216646101 + 0.8252425506i & -0.1613739097 - 0.3128773077i & 0.321129708 + 0.2776948279i \\ -0.1802697442 - 0.1287928363i & 0.1140421168 - 0.6235401084i & 0.2988391186 - 0.6780874093i \\ -0.0807466501 - 0.4985656009i & -0.6396895224 - 0.2550601797i & 0.3406188724 + 0.3932336755i \end{bmatrix}$$

$$S = \begin{bmatrix} 3.4167487815 & 0 \\ 0 & 1.9751666399 \\ 0 & 0 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.8073630659 & 0.5900549803 \\ -0.5677972825 + 0.1605338775i & 0.7769082036 - 0.2196560114i \end{bmatrix}$$

$$SS^\dagger = \begin{bmatrix} 11.67417224 & 0 & 0 \\ 0 & 3.90128326 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

[11]:
```
# Perform the multiplication U * S * V^dagger
A_recons = U @ S @ V.getH()

# Display the result
#display(array_to_latex(A_reconstructed, prefix='U S V^\\dagger = '))

np.allclose(A, A_recons)
```

[11]:
```
True
```

Operator trace

«<

Definition: The trace of an operator A is defined as the sum

$$\mathrm{tr}A = \sum_i \langle e_i|A|e_i\rangle = \sum_i A_{ii}$$

of its diagonal matrix elements in any orthonormal basis $\{|e_i\rangle\}$

To be consistent, this definition requires proving that the choice of basis does not matter.

Lemma: the trace of an operator is independent of the basis in which it is calculated.

Proof

$$
\begin{aligned}
\mathrm{tr}A &= \sum_i A_{ii} = \sum_i \langle i|A|i\rangle = \sum_i \langle i|A\left(\sum_j |\tilde{j}\rangle\langle\tilde{j}|\right)|i\rangle \\
&= \sum_{ij} \langle i|A|\tilde{j}\rangle\langle\tilde{j}|i\rangle = \sum_{ij}\langle\tilde{j}|i\rangle\langle i|A|\tilde{j}\rangle \\
&= \sum_j \langle\tilde{j}|\left(\sum_i |i\rangle\langle i|\right)A|\tilde{j}\rangle = \sum_j \langle\tilde{j}|A|\tilde{j}\rangle \\
&= \sum_j \tilde{A}_{jj} \qquad (19)
\end{aligned}
$$

By this important property, the trace of A coincides with the sum of its eigenvalues:

$$
\mathrm{tr}\, A = \sum_i \langle\lambda_i|A|\lambda_i\rangle = \sum_i \lambda_i
$$

provided that A is diagonalizable in the basis $\{|\lambda_i\rangle\}$.

$$
A|\lambda_j\rangle = \lambda_i|\lambda_i\rangle
$$

The trace enjoy a series of important properites

- It is al linear function
$$
\mathrm{tr}(A+B) = \mathrm{tr}A + \mathrm{tr}B
$$
- It is symmetric
$$
\mathrm{tr}\, AB = \mathrm{tr}\, BA
$$
  From here the cyclicity follows immediately
$$
\mathrm{tr}\, AB...C = \mathrm{tr}\, A(B...C) = \mathrm{tr}\,(B...C)A = \mathrm{tr}\, B...CA
$$
- Let the operator \$A = | u$\rangle\langle v|$\$then, foranyoperator\$B\$itholdsthat $\mathrm{tr}\left(B|u\rangle\langle v|\right) = \sum_i \langle e_i|B|u\rangle\langle v|e_i\rangle = \langle v|\left(\sum_i |e_i\rangle\langle e_i|\right)B|u\rangle = \langle v|B|u\rangle$

2.1.8 Lin($\mathcal{H}$) as a Hilbert space

To transform \$Lin(H)\$ into a Hilbert space it is only necessary to define a Hermitian inner product In a basis we have that

$$
(A,B) = \sum_{ij} A^\dagger_{ij} B_{ji} = \sum_{ij} A^*_{ji} B_{ji}
$$

whereas

$$(B, A) = \sum_{ij} B^\dagger_{ij} A_{ji} = \sum_{ij} B^*_{ji} A_{ji} = \sum_{ij} A_{ji} B^*_{ji}$$

It follows that $(B,A) = (A,B)^*$. Moreover, it is trivial to check that $(A,B+C) = (A,B) + (A,C)$, so it is a sesquilinear or Hermitian inner product.

2.1.9 Operator norm and distance

A **norm** defined on $Lin(H)$ is a real function $A \rightarrow |A| \in \mathbb{R}$ $withthepropertiesthatweredefinedina$ $previoussection$

The seemeingly weird appearance of the factor p is arrange so that homogeneity of degree one is achieved

$$\|\lambda A\|_p = \lambda \|A\|_p$$

The three most frequent cases are

- **Trace norm**

$$p = 1 \quad \Rightarrow \quad |A|_1 = \mathrm{tr}\sqrt{A^\dagger A}$$

This norm is equal to the sum of the singular values of $A \;\Rightarrow\; |A|_1 = \sum_i^r s_i$, where s_i^2 are the eigenvalues of $A^\dagger A$.

- **Frobenius norm**

$$p = 2 \quad \Rightarrow \quad |A|_2 = \sqrt{\mathrm{tr} A^\dagger A}$$

The Frobenius norm is the one naturally derived from the inner product $\quad |A|_2 = \sqrt{(A, A)}$

- **Spectral norm**

$$p = \infty \quad \Rightarrow \quad |A|_\infty = \lim_{p\to\infty} |A|_p$$

It can be shown that the spectral norm is equivalent to the following definition

$$|A|_\infty = \max_{|u\rangle \in \mathcal{H}} \{ \|A|u\rangle\| \quad \text{with} \; \||u\rangle\| = 1\}$$

Ejercicio 1.3.10

write, in python, a function _() , that calculates the trace norm of an operator.

2.1.10 Trace distance

Any norm allows one to define a notion of *distance* or *difference* between two operators.

Linear maps

«<

Linear maps form themselves a vector space $\mathcal{E} \in T(\mathcal{H}_1, \mathcal{H}_2)$.

Classes of linear maps

- **Trace preserving map**

$\mathcal{E}$ is *trace preserving* map if, for any $A \in U$

$$Tr(\mathcal{E}(A)) = Tr(A)$$

- **Positive map**

Remember that $\mathrm{Pos}(\mathcal{H}) \subset \mathrm{Lin}(\mathcal{H})$ is the subset of *positive semi-definite linear* operators on a Hilbert space $\mathcal{H}$

$$A \in \mathrm{Pos}(U) \Leftrightarrow \langle\psi|A\psi\rangle \geq 0 \qquad \forall\psi \in U$$

$\mathcal{E} \in T(\mathcal{H}_1, \mathcal{H}_2)$ is a *positive linar map* if it maps

$$A \in \mathrm{Pos}(\mathcal{H}_1) \rightarrow \mathcal{E}(A) \in \mathrm{Pos}(\mathcal{H}_2)$$

- **Hermiticity preserving maps**

$\mathcal{E} \in T(\mathcal{H}_1, \mathcal{H}_2)$ is an *hermiticity preserving map* if and only if it maps the subspaces of hermitian operators $\mathrm{Her}(\mathcal{H}) \in \mathrm{Lin}(\mathcal{H})$

$$A \in \mathrm{Her}(\mathcal{H}_1) \rightarrow \mathcal{E}(A) \in \mathrm{Her}(\mathcal{H}_2)$$

Functions of Operators

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Functions of operators are, in general non-linear maps $f : \mathrm{Lin}(\mathcal{H}) \rightarrow \mathrm{Lin}(\mathcal{H})$ which are defined after some complex valued function $f(z) : \mathbb{C} \rightarrow \mathbb{C}$.

Analytic functions

We are used to writing functions *of a real or complex variable*. For example $f(x)= xˆ2$, or $ f(z) = eˆz$.

We would like to give meaning to the function *of an operator* $ A $\rightarrow f(A)$$

In the case that $f(z)$ is an analytic function expressible as a Taylor series around $x=0$

$$f(z) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0)\, z^n$$

we will take as **definition** the *same series* changing the argument $x\to A$

$$f(A) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0)\, A^n$$

`<b>Note:</b>`

1. In the same way that, for analytic functions, $f(z)^* = f(z^*)$, the above definition also ensures that $f(A)^\dagger = f(A^\dagger)$

2.1.11 Exponential of an operator

the exponential of a function $z \to e^z$ motivates the analogous definition of *exponential of an operator*

$$\exp(A) = e^A = I + A + \frac{1}{2}A^2 + \frac{1}{3!}A^3 + ...$$

An important property of the exponential $e^x e^y = e^{x+y}$, **does not** translate in general to operators.

It will be *only true when they commute with each other.*

For the generic case we have two options to work around

We see that

- If A and B commute,

$[A, B] = 0 \;\Leftrightarrow\; e^A e^B = e^{A+B}$

- If the commutator of A and B is a c-number

$$[A, B] = cI \;\Leftrightarrow\; e^A e^B = e^{A+B} e^{\frac{c}{2}}$$

- The inverse of e^A is e^{-A}

$$[A, A] = 0 \Rightarrow e^A e^{-A} = e^{A-A} = e^0 = I$$

The converse of the BCH formula is the *Zassenhaus expression*

$$e^{A+B} \;=\; e^A e^B e^{-\frac{1}{2}[A,B]} e^{\frac{1}{6}\left(2[B,[A,B]]+[A,[A,B]]\right)} \dots$$

Where the dots involve exponentials of higher nested operators. This leads easily to the following theorem

Proof

Using the BCH formula

$$\lim_{n\to\infty}\left(e^{A/n}e^{B/n}\right)^n = \lim_{n\to\infty}\left(e^{\left(A/n+B/n+\frac{1}{2}[A,B]/n^2+\frac{1}{12}[A,[A,B]]/n^3+\frac{1}{12}[B,[B,A]]/n^3+...\right)}\right)^n \tag{20}$$

$$= \lim_{n\to\infty}\left(e^{\left(A+B+\frac{1}{2}[A,B]/n+\frac{1}{12}[A,[A,B]]/n^2+\frac{1}{12}[B,[B,A]]/n^3+...\right)}\right) \tag{21}$$

$$= e^{(A+B)} \tag{22}$$

2.1.12 Unitary operators from Hermitian ones

Every unitary operator U can be expressed as the imaginary exponential of a Hermitian operator H

$$U = e^{iH}$$

Indeed,

$$\begin{aligned}
U^\dagger &= \left(e^{iH}\right)^\dagger = \left(1 + iH + \frac{1}{2}(iH)^2 + ...\right)^\dagger && (23)\\
&= 1 - iH^\dagger + \frac{1}{2}(-i)^2(H^2)^\dagger + ... && (24)\\
&= 1 - iH + \frac{1}{2}H^2 - ... && (25)\\
&= e^{-iH} && (26)\\
&= U^{-1} && (27)
\end{aligned}$$

therefore, U is unitary if and only if H is Hermitian.

Euler operator formula

Proof:

$$\begin{aligned}
e^{i\alpha A} &= I + i\alpha A + \frac{1}{2}(i\alpha A)^2 + \frac{1}{3!}(i\alpha A)^3 + ...\\
&= I + i\alpha A - \frac{1}{2}\alpha^2 I - i\frac{1}{3!}\alpha^3 A + ...\\
&= \left(1 - \frac{1}{2}\alpha^2 + ...\right) I + i\left(\alpha - \frac{1}{3!}\alpha^3 + ...\right) A\\
&= \cos\alpha I + i\sin\alpha A
\end{aligned}$$

General functions

No always $F(z)$ is an analitic function around z_0. For example $f(z) = \exp(1/z)$ around $z_0 = 0$. Hence, this function cannot be defined through its Taylor expansion.

Still, if the function $f(z)$ exists, $f(A)$ will also exist. The proper way to define it is by resorting to the *diagonalized form* of A.

In other words, if the matrix $A_{ij}^{(D)} = \lambda_i \delta_{ij}$ is diagonal, any function of it is, trivially, the diagonal matrix obtained by evaluating \$f(λ_i)\$

$$f(A_{ij}^{(D)}) = \begin{bmatrix} f(\lambda_1) & & & \\ & f(\lambda_2) & & \\ & & \ddots & \\ & & & f(\lambda_n) \end{bmatrix}$$

Example 1:

$$e^{1/A} = \sum_i e^{1/\lambda_i} |\lambda_i\rangle\langle\lambda_i|$$

Example 2:

$$\mathrm{tr}(A \log A) \quad = \quad \mathrm{tr}\left[\left(\sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j|\right)\left(\sum_k \log\lambda_k |\lambda_k\rangle\langle\lambda_k|\right)\right] \quad = \quad \mathrm{tr}\left[\sum_k \lambda_k \log\lambda_k |\lambda_k\rangle\langle\lambda_k|\right] \tag{28}$$

$$= \quad \mathrm{tr}\begin{bmatrix} \lambda_1\log\lambda_1 & & & \\ & \lambda_2\log\lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n\log\lambda_n \end{bmatrix} = \sum_k \lambda_k \log\lambda_k \tag{29}$$

\# Pauli matrices

«<

Hermitian matrices form a vector subspace \$Her(H)⊂ Lin($\mathcal{H}$)\$$thatadmitsabasisofHermitianmatrices.$

Note: integer subscripts are also used. $\sigma_1 = \sigma_x,\ \sigma_2 = \sigma_y$ y $\sigma_3 = \sigma_z$.

- If we add the identity matrix $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, the set $\{I, \sigma_x, \sigma_y, \sigma_z\}$ forms a *basis* for the space of *Hermitian matrices* \$2×2\$.

$$A = a_0 I + \mathbf{a}\cdot\boldsymbol{\sigma} \quad = \quad a_0 I + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3 = \begin{bmatrix} a_0 + a_3 & a_1 - ia_2 \\ a_1 + ia_2 & a_0 - a_3 \end{bmatrix} = A^\dagger \tag{30}$$

with $a_\mu = (a_0, a_1, a_2, a_3) \in \mathbb{R}$ four real numbers

- Pauli matrices enjoy three properties that make them rather unique
  - hermiticity $\sigma_i^\dagger = \sigma_i$

– unitarity $\sigma_i^\dagger = \sigma_i^{-1} = \sigma_i$

– traceless $\mathrm{tr}(\sigma_i) = 0$

Pauli algebra

The composition of two Pauli matrices is another Pauli matrix that satisfies the following identity

$$\sigma_i\sigma_j = \delta_{ij} I + i\epsilon_{ijk}\sigma_k$$

where

$$\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1 \quad , \quad \epsilon_{213} = \epsilon_{132} = \epsilon_{321} = -1$$

Examples:

$$\begin{aligned}
\sigma_1\sigma_2 &= i\sigma_3 && (31)\\
\sigma_2\sigma_1 &= -i\sigma_3 && (32)\\
\sigma_2\sigma_1\sigma_2 &= \sigma_2(i\sigma_3) = i^2\sigma_1 = -\sigma_1 && (33)\\
\sigma_2\sigma_2 &= I && (34)
\end{aligned}$$

[12]:
```
s0 = np.matrix([[1,0],[0,1]])
s1 = np.matrix([[0,1],[1,0]])
s2 = np.matrix([[0,-1j],[1j,0]])
s3 = np.matrix([[1,0],[0,-1]])


'verify all the options'
print(s1*s1==s0)
print(s1*s2==1j*s3)
print(s2*s1==-1j*s3)
print(s2*s1*s2==-s1)
print(s1*s1==s0)
```

```
[[ True  True]
 [ True  True]]
[[ True  True]
 [ True  True]]
[[ True  True]
 [ True  True]]
[[ True  True]
 [ True  True]]
[[ True  True]
 [ True  True]]
```

Notes: from the previous composition relations the following (anti)commutation rules immediately follow

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij} \qquad , \qquad [\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$$

Taking the trace of the composition relation we obtain

$$\mathrm{tr}(\sigma_i\sigma_j) = \mathrm{tr}(\delta_{ij}I + i\epsilon_{ijk}\sigma_k) = \delta_{ij}\,\mathrm{tr}I + i\epsilon_{ijk}\,\mathrm{tr}\sigma_k = 2\delta_{ij}$$

This allows to endow the algebra of Pauli mátrices with a scalar product, under which they are orthonormal

$$(\sigma_i, \sigma_j) \equiv \frac{1}{2}\mathrm{tr}(\sigma_i\sigma_j) = \delta_{ij}$$

This can be enhanced to the set $\sigma_\mu = (\sigma_0, \sigma_1, \sigma_2, \sigma_3)$ as

$$(\sigma_\mu, \sigma_\nu) \equiv \frac{1}{2}\mathrm{tr}(\sigma_\mu\sigma_\nu) = \delta_{\mu\nu}$$

So if $A = \sum_\mu a_\mu\sigma_\mu$ we may recover the coefficients a_μ thanks to this scalar product

$$\begin{aligned}
(A, \sigma_\mu) &= \frac{1}{2}\mathrm{tr}\,A\sigma_\mu = \frac{1}{2}\mathrm{tr}\big(\sum_\nu a_\mu\sigma_\nu\big)\sigma_\mu && (35)\\
&= \sum_\nu a_\nu \frac{1}{2}\mathrm{tr}\,(\sigma_\mu\sigma_\nu) = \sum_\nu a_\nu\delta_{\nu\mu} && (36)\\
&= a_\mu && (37)
\end{aligned}$$

2.2 Exponentiation

Let us consider the most general 2×2 Hermitian matrix

$$A = a_0 I + \mathbf{a}\cdot\boldsymbol{\sigma} \qquad (38)$$

with $a_\mu \in \mathbb{R}$.

We would like to find an analytic expression for e^{iA} in terms of $(a_0, \mathbf{a})$

Separate ${**a**}$ **into a modulus,** $a = |\mathbf{a}| = \sqrt{a_1^2 + a_2^3 + a_3^2}$ **, and a unit direction vector** $\hat{\mathbf{n}} = \mathbf{a}/a$

$$\mathbf{a} = (a_1, a_2, a_3) = a\left(\frac{a_1}{a}, \frac{a_2}{a}, \frac{a_3}{a}\right) = a\,\hat{\mathbf{n}}$$

Then

$$A = a_0 I + \mathbf{a}\cdot\boldsymbol{\sigma} = a_0 I + a\,(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})$$

Proof:

The operator $ $\cdot\boldsymbol{\sigma}\$verifies(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})^2 = I$. Let us check

$$(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})^2 = n_i n_j \sigma_i \sigma_j = n_i n_j (\delta_{ij} I + i\epsilon_{ijk}\sigma_k) = \sum_i (n_i)^2 I$$

since $n_i n_j$ is symmetric under exchange of i, j while ϵ_{ijk} is antisymmetric. The lemma follows from a previous theorem for the Euler operator formula.

This generalizes Euler's formula for a complex phase.

$$e^{i\alpha} = \cos\alpha + i\sin\alpha$$

The final expression for

$$e^{iA} = e^{i(a_0 I + \mathbf{a}\cdot\boldsymbol{\sigma})} = e^{i\alpha_0}\big(\cos a\, I + i\sin a\,(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})\big)$$

Exercise 1.3.12

Obtain the spectral decomposition of the three Pauli matrices, \$σ_x, σ_y\$ and \$σ_z\$.

Use this decomposition to prove that

$$e^{i\alpha\,\mathbf{n}\cdot\boldsymbol{\sigma}} = \cos\alpha\, I + i\sin\alpha\,\mathbf{n}\cdot\boldsymbol{\sigma}$$

[13]:
```
from scipy.linalg import expm



avec = np.random.rand(3)
a = np.linalg.norm(avec)
nvec = avec/a
print('a=',a)
display(array_to_latex(nvec))

sigvec = np.array([s1,s2,s3])



adots= sum(list(avec[i]*sigvec[i] for i in range(3)))

'exponentiating'
e1 = expm(1j*adots)

'using the Euler-like formula'
ndots= sum(list(nvec[i]*sigvec[i] for i in range(3)))
e2 = np.cos(a)*s0 + 1j*np.
↪sin(a)*(nvec[0]*sigvec[0]+nvec[1]*sigvec[1]+nvec[2]*sigvec[2])

'verify'
```

```
display(array_to_latex(e1,prefix='exp(s1)='))
display(array_to_latex(e2,prefix='exp(s1)='))
```

```
a= 1.193860017140821
```

$$\begin{bmatrix} 0.3633607915 & 0.4809988904 & 0.7978778118 \end{bmatrix}$$

$$exp(s1) = \begin{bmatrix} 0.3680735922 + 0.7418641253i & 0.4472311622 + 0.3378516507i \\ -0.4472311622 + 0.3378516507i & 0.3680735922 - 0.7418641253i \end{bmatrix}$$

$$exp(s1) = \begin{bmatrix} 0.3680735922 + 0.7418641253i & 0.4472311622 + 0.3378516507i \\ -0.4472311622 + 0.3378516507i & 0.3680735922 - 0.7418641253i \end{bmatrix}$$