UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

Operators (functions and operations)

OPERATORS in quatum mechanics

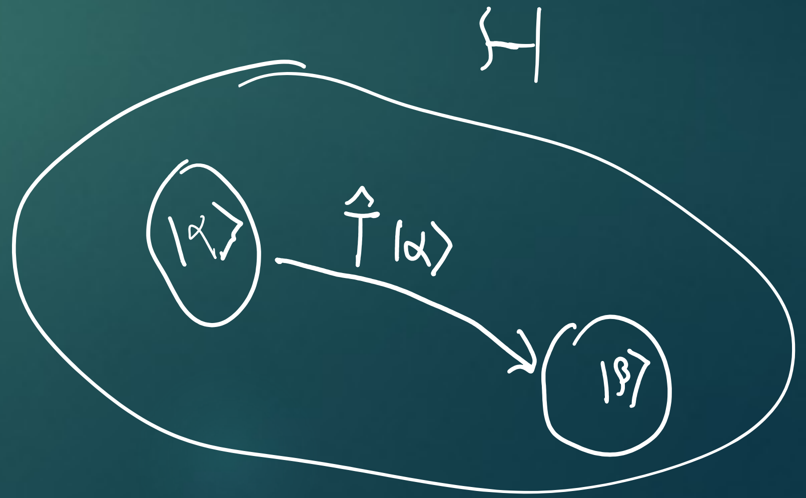
- An **operator** is a “rule” prescribing how to change one vector $|\boldsymbol{\alpha}\rangle$ of a linear vector space $\boldsymbol{\mathcal{H}}$, into another abstract vector, $|\beta\rangle$ of the same or a different vector space

$$|\beta\rangle = \hat{T}|\alpha\rangle$$

*note that $\hat{T}$ acts on $|\alpha\rangle$ (right side) and is place close to the vertical line of the ket

- A <u>linear</u> operator can be also seen as a linear function which maps $\boldsymbol{\mathcal{H}}$ into itself. In other words, to each $|\boldsymbol{\alpha}\rangle$ in $\boldsymbol{\mathcal{H}}$, $\hat{T}$ assigns another element $\hat{T}|\alpha\rangle$ in $\boldsymbol{\mathcal{H}}$ in such a way that:

$$\hat{T}\,(a|\alpha\rangle + b|\gamma\rangle) = a\hat{T}|\alpha\rangle + b\hat{T}|\gamma\rangle$$



OPERATORS in quatum mechanics

Examples of operators:

- *Identity operator* $|\alpha\rangle = \hat{I}|\alpha\rangle$
- Differentiation operator $g(x) = \widehat{D}|f\rangle \equiv \frac{df}{dx}$
- Gradient operator $\vec{\nabla} f(x, y, z) = \boldsymbol{e}_x \delta f / \delta x + \boldsymbol{e}_y \delta f / \delta y + \boldsymbol{e}_z \delta f / \delta z$

- It also possible to define an operator acting on a bra vector by making the Hermitian conjugation of $|\beta\rangle = \hat{T}|\alpha\rangle$:

$$\langle\beta| = \langle\boldsymbol{\alpha}|\, \hat{T}^{\dagger}$$

You may note that the operator is applied to the right of the bra (still closer to the vertical line)…

Why?

OPERATORS in quatum mechanics

- It also possible to define an operator acting on a bra vector by making the Hermitian conjugation of $|\beta\rangle = \hat{T}|\alpha\rangle$:

$$\langle\beta| = \langle\boldsymbol{\alpha}|\,\hat{T}^\dagger$$

$$\begin{bmatrix} t_{11} & t_{12} & \cdots & t_{1N} \\ \vdots & & & \vdots \\ t_{N1} & \cdots & & t_{NN} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{bmatrix}$$

$N \times N \quad N \times 1 \quad N \times 1$

$$[N \times M]\,[M \times L] = [N \times L]$$

You may note that the operator is applied to the right of the bra (still closer to the vertical line)…

Why?

$$\underbrace{[a_1^* \; a_2^* \; a_N^*]}_{1 \times N} \begin{bmatrix} \\ T^\dagger \\ \\ \end{bmatrix} = \underbrace{[b_1^* \; b_2^* \; b_N^*]}_{1 \times N}$$

$\langle\alpha| \qquad \underline{N \times N} \qquad \langle\beta|$

OPERATORS in quatum mechanics

- So $|\beta\rangle = \hat{T}|\alpha\rangle$ and $\langle\beta| = \langle\boldsymbol{\alpha}|\,\hat{T}^{\dagger}$

$$\begin{bmatrix} t_{11} & t_{12} & \cdots & t_{1N} \\ \vdots & & & \vdots \\ t_{N1} & \cdots & \cdots & t_{NN} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_M \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_M \end{bmatrix}$$

$$\begin{bmatrix} a_1^* & a_2^* & \cdots & a_M^* \end{bmatrix} \begin{bmatrix} T^{\dagger} \end{bmatrix} = \begin{bmatrix} b_1^* & b_2^* & \cdots & b_M^* \end{bmatrix}$$

$$b_1 = t_{11}a_1 + t_{12}a_2 + t_{1N}a_N$$

$$b_1^* = t_{11}^* a_1^* + t_{12}^* a_2^* + t_{1N}^* a_N^*$$

$$\Rightarrow \begin{bmatrix} a_1^* & a_2^* & \cdots & a_M^* \end{bmatrix} \begin{bmatrix} t_{11}^* & \cdots \\ t_{12}^* & \cdots \\ t_{1N}^* & \cdots \end{bmatrix} = \begin{bmatrix} b_1^* & b_2^* & \cdots & b_M^* \end{bmatrix}$$

$$T^{\dagger} = (T^*)^T$$

OPERATORS in quatum mechanics

- So, we confirmed the “formal” rule of Hermitian conjugation of a matrix by the “operational” rule of the Hermitian conjugation of the matrix operator

$$T^\dagger = (T^*)^T$$

OPERATORS in quatum mechanics

- It also possible to define an operator acting on a bra vector by making the Hermitian conjugation of $|\beta\rangle = \hat{T}|\alpha\rangle$:

$$\langle\beta| = \langle\boldsymbol{\alpha}|\,\hat{T}^{\dagger}$$

In this case we know how to make the Hermitian conjugate of the matrix, hence of the matrix operator $\hat{T}$, but in general <u>we do not have any clue</u> except for the <u>definition of inner product</u>, that we may use to get an expression of $\hat{T}$

So, I will make the inner product between $|\boldsymbol{\beta}\rangle$ and $\hat{\boldsymbol{T}}|\boldsymbol{\alpha}\rangle$

OPERATORS in quatum mechanics

The inner product will be: $(|\beta\rangle)^{\dagger}\,\hat{T}|\alpha\rangle = \langle\beta|\hat{T}|\alpha\rangle$

which is often called as a matrix element

…but we know that $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^{*}$

note that

$\langle\beta|\alpha\rangle^{\dagger} = \langle\beta|\alpha\rangle^{*}$

Because it is a scalar!

OPERATORS in quatum mechanics

The inner product will be: $(|\beta\rangle)^{\dagger}\,\hat{T}|\alpha\rangle = \langle\beta|\hat{T}|\alpha\rangle$
which is often called as a matrix element

…but we know that $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^{*}$

so: $\langle\beta|\hat{T}|\alpha\rangle^{*} = \langle\alpha|\,\hat{T}^{\dagger}|\beta\rangle$

By using this equation, we can get $\hat{T}^{\dagger}$

OPERATORS in quatum mechanics

Let's see an example

$$\boxed{\hat{D}|f\rangle \equiv \frac{df}{dx}}$$

$\rightarrow$ but $\hat{D}^{+}$?

OPERATORS in quatum mechanics

N.B.: Integration by parts

$$\int g(x) \underbrace{f'(x)}_{= \frac{df(x)}{dx}} dx = g(x)\, f(x) - \int f(x)\, g'(x$$

OPERATORS in quatum mechanics

Let's see an example

$$\boxed{\hat{D}|f\rangle \equiv \frac{df}{dx}}$$

→ but $\hat{D}^{+}$?

we can make inner product

integration by part

$$\langle g|\hat{D}|f\rangle^{*} \equiv \int_{-\infty}^{\infty} g^{*}(x)\, \underbrace{\frac{df}{dx}}_{\text{correspond to } \hat{D}|f\rangle} dx = g^{*}(x) f(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f(x)\, \frac{dg^{*}(x)}{dx}\, dx$$

must vanish at $\pm\infty$ because square-integrable

$$= -\int_{-\infty}^{\infty} f(x)\, \frac{dg^{*}(x)}{dx}\, dx$$

OPERATORS in quatum mechanics

Let's see an example

$$\langle g|\hat{D}|f\rangle = -\int_{-\infty}^{\infty} f(x)\,\frac{dg^*(x)}{dx}\,dx$$

We know

$$\langle g|\hat{D}|f\rangle^* = \langle f|\hat{D}^\dagger|g\rangle = -\int_{-\infty}^{\infty} f^*(x)\,\frac{dg(x)}{dx}\,dx$$

OPERATORS in quatum mechanics

Let's see an example

$$\langle g|\hat{D}|f\rangle = -\int_{-\infty}^{\infty} f(x)\,\frac{dg^*(x)}{dx}\,dx$$

We know

$$\langle g|\hat{D}|f\rangle^* = \langle f|\hat{D}^\dagger|g\rangle = -\int_{-\infty}^{\infty} f^*(x)\,\frac{dg(x)}{dx}\,dx$$

$$\hat{D}^\dagger = -\frac{d}{dx}$$

OPERATORS in quatum mechanics

- Very important definition:

if $\langle\beta|\hat{T}|\alpha\rangle^* = \langle\alpha|\hat{T}|\beta\rangle$

and so $\hat{T}^\dagger = \hat{T}$ (an operator and its Hermitian conjugate are equal)

The operator is called **Hermitian operator** (or self-adjoint)

Such operators have important properties that will be discussed later…

OPERATORS (functions and operations)

- The collection of all operators is itself a linear space, since a scalar times an operator (a · $\hat{T}$) is an operator, and the sum of two operators is also an operator

The operator (a $\hat{T}$ + b $\hat{S}$) applied to an element $|\, \alpha \,\rangle$ of $\mathcal{H}$ yields the result:

$$(a\, \hat{T} + b\, \hat{S})|\alpha\rangle = a\, \hat{T}|\alpha\rangle + b\, \hat{S}|\alpha\rangle$$

OPERATORS (functions and operations)

- The product $\hat{T}\,\hat{S}$ of two operators $\hat{T}$ and $\hat{S}$ is the operator obtained by first applying $\hat{S}$ to some ket, and then $\hat{T}$ to the ket which results from applying $\hat{S}$:

$$(\hat{T}\,\hat{S})|\alpha\rangle = \hat{T}\,(\,\hat{S}|\alpha\rangle\,)$$

Of course, in case of bra vector, the order will be opposite:

$$\langle\alpha|(\hat{T}\,\hat{S}) = (\,\langle\alpha|\,\hat{T}\,)\,\hat{S}$$

OPERATORS (functions and operations)

The product $\hat{T}\,\hat{S}$ of two operators $\hat{T}$ and $\hat{S}$ is the operator obtained by first applying $\hat{S}$ to some ket, and then $\hat{T}$ to the ket which results from applying $\hat{S}$:

$$(\hat{T}\,\hat{S})|\alpha\rangle = \hat{T}\,(\,\hat{S}|\alpha\rangle\,)$$

- Thus, it is evident that **operator multiplication**, unlike multiplication of scalars, <u>**is not commutative,**</u> and in general: $\hat{T}\,\hat{S} \neq \hat{S}\hat{T}$

OPERATORS (functions and operations)

- In the <u>exceptional</u> case in which

$$\hat{T}\,\hat{S} = \hat{S}\hat{T}$$

one says that these two operators <u>**commute**</u>

In general, we can define the <u>**commutator**</u> of two operators:

$$[\hat{T},\hat{S}] = \hat{T}\,\hat{S} - \hat{S}\hat{T}$$

The commutator is often the <u>most important information</u> that you can have about the two operators

OPERATORS (functions and operations)

We have seen the identity operator $\hat{I}$: $|\alpha\rangle = \hat{I}|\alpha\rangle$

- We can then define the inverse operator $\hat{T}^{-1}$:

$$\hat{T}^{-1}\,\hat{T} = \hat{T}\,\hat{T}^{-1} = \hat{I}$$

And thus:

If $\hat{T}|\alpha\rangle = |\beta\rangle$

Then $|\alpha\rangle = \hat{T}^{-1}\,|\beta\rangle$

OPERATORS (functions and operations)

We have seen the identity operator $\hat{I}$: $\quad |\alpha\rangle = \hat{I}|\alpha\rangle$

- We can then define the inverse operator $\hat{T}^{-1}$:

$$\hat{T}^{-1}\,\hat{T} = \hat{T}\,\hat{T}^{-1} = \hat{I} \equiv \begin{bmatrix} 1 & 0 & \cdots & 0 \\ \vdots & 1 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

$$I_{ij} \equiv \delta_{ij}$$

A matrix has an inverse if and only if its determinant is nonzero, in fact:

$$\hat{T}^{-1} = \frac{1}{det\hat{T}} C^{T}$$

where C is the matrix of cofactors

OPERATORS (functions and operations)

One can easily show that

$$(\hat{T}\hat{S})^{\dagger} = \hat{S}^{\dagger}\,\hat{T}^{\dagger}$$

Then, if the two Operators are Hermitian:

$$(\hat{T}\hat{S})^{\dagger} = \hat{S}\,\hat{T}$$

But in that case:

$$[\hat{T},\hat{S}]^{\dagger} = \left(\hat{T}\hat{S} - \hat{S}\hat{T}\right)^{\dagger} = \left(\hat{T}\hat{S}\right)^{\dagger} - \left(\hat{S}\hat{T}\right)^{\dagger} = \hat{S}\,\hat{T} - \hat{T}\hat{S} = -\,[\hat{T},\hat{S}]$$

Operators that change sign upon Hermitian conjugation are anti-Hermitian

Thus, the commutator of two Hermitian Operators is <u>anti-Hermitian</u>

OPERATORS (functions and operations)

$[\hat{T},\hat{S}]^{\dagger}$= - $[\hat{S},\hat{T}]$

N.B. The commutator of two Hermitian Operators is anti-Hermitian

Let's put $[\hat{T},\hat{S}]$ = -$\hat{B}$

Then $\hat{B}$ is anti-Hermitian and :

$\hat{B}^{\dagger}$= -$\hat{B}$

If $\hat{A}$= $i\hat{B}$ then: $\hat{A}^{\dagger}$= -$i\hat{B}^{\dagger}$= $i\hat{B}$=$\hat{A}$ thus $\hat{A}$ must be Hermitian.

Hence: $[\hat{T},\hat{S}]$= $i\hat{A}$

If the commutator is a number: $[\hat{T},\hat{S}]$= ia

Where **a** is real.

We could consider **a** as a vector, hence $\hat{A}$ will represent a real function, and it is Hermitian.

OPERATORS (functions and operations)

We could consider **a** as a vector, hence $\hat{A}$ will represent a real function, and it is Hermitian.

For the same reason:

the potential V(x),

which can be represented by an operator $\hat{V}$ (diagonal matrix),

if it is a real function, then its corresponding operator is Hermitian.

OPERATORS (functions and operations)

The potential V(x),

which can be represented by an operator $\hat{V}$ (diagonal matrix),

if it is a real function, then its corresponding operator is Hermitian.

We have seen that the differential operator $\hat{D}$ is anti-Hermitian.

But one can easily prove that $i\frac{d}{dx}$ is Hermitian

Also $\frac{d^2}{dx^2}$ is Hermitian, thus also the operator $\boldsymbol{\nabla}^{\mathbf{2}}$ is Hermitian.

Thus, $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathrm{r})$ is Hermitian

Eigenvalues and Eigenvectors

In general we have seen that the result of an operator applied to a vector is another different vector.

There is a class of vectors, called eigenvectors, that are not much changed by some operators, but they are multiplied by a number (called eigenvalue)

$$\hat{T}|\alpha\rangle = \lambda_\alpha|\alpha\rangle$$

- For each eigenvector there might be one and only one corresponding eigenvalue.
- For each eigenvalue we may have more than one corresponding eigenvector.
- If for each eigenvalue there exists only a single eigenvector, we describe this eigenvalue as **non-degenerate**
- If several eigenvectors correspond to the same eigenvalue, the respective eigenvalue is naturally called "**degenerate**"
- Any (nonzero) multiple of an eigenvectors still an eigenvector with the same eigenvalue

Eigenvalues and Eigenvectors

Eigenvector equation: $\hat{T}|\alpha\rangle = \lambda_\alpha|\alpha\rangle$

- With respect to a particular basis $|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \ldots + a_n|e_n\rangle$

the eigenvector equation assumes the matrix form:

$$\hat{T}\boldsymbol{a} = \lambda\,\boldsymbol{a}$$ (with nonzero **a** vector)

$$(\hat{T} - \lambda\mathbf{I})\boldsymbol{a} = \mathbf{0}$$ (**0** is the zero matrix)

And because a may not be 0 by assumption, then the determinant of $(\hat{T} - \lambda\mathbf{I})$ must be 0:

$$\det(\hat{T} - \lambda\mathbf{I}) = \mathbf{0}$$

Eigenvalues and Eigenvectors

Because a may not be 0 by assumption, then the determinant of $(\hat{T}-\lambda\mathbf{I})$ must be 0:

$$\det(\hat{T}-\lambda\mathbf{I})=\begin{vmatrix} T_{11}-\lambda & T_{12} & \cdots & T_{1n} \\ T_{21} & T_{22}-\lambda & \cdots & T_{2n} \\ \vdots & \vdots & & \vdots \\ T_{n1} & T_{n2} & \cdots & T_{nn}-\lambda \end{vmatrix}=\mathbf{0}$$

Expansion of the determinant yields an algebraic equation for λ :

$$C_n\lambda^n + C_{n-1}\lambda^{n-1} + \cdots + C_1\lambda + C_0$$

This is called the **characteristic equation** for the matrix allowing to calculate the eigen-values.

To construct the corresponding eigenvectors one should plug each $\boldsymbol{\lambda}$ back into equation $\hat{T}\boldsymbol{a} = \lambda\,\boldsymbol{a}$ and solve for the components of a.

Eigenvalues and Eigenvectors

Find the eigenvalues and eigenvectors of the following matrix: :

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

$$(M-\lambda I) = \begin{pmatrix} 2-\lambda & 0 & -2 \\ -2i & i-\lambda & 2i \\ 1 & 0 & -1-\lambda \end{pmatrix}$$

$$\det(M-\lambda I)=0$$

characteristic equation

Eigenvalues and Eigenvectors

$$\det(M - \lambda I) = \begin{vmatrix} 2-\lambda & 0 & -2 \\ -2i & i-\lambda & 2i \\ 1 & 0 & -1-\lambda \end{vmatrix}$$

$$= (2-\lambda)(i-\lambda)(-1-\lambda) - (-2)(i-\lambda)$$

$$= (2i - \lambda i - 2\lambda + \lambda^2)(-1-\lambda) + 2i - 2\lambda$$

$$= \cancel{-2i} + \lambda i + \cancel{2\lambda} - \lambda^2 - 2i\lambda + \lambda^2 i + 2\lambda^2 - \lambda^3 + \cancel{2i} - \cancel{2\lambda}$$

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

$$\lambda_1 = 0, \quad \lambda_2 = 1, \quad \lambda_3 = i$$

Eigenvalues and Eigenvectors

$$\det(M-\lambda I)=\begin{vmatrix} 2-\lambda & 0 & -2 \\ -2i & i-\lambda & 2i \\ 1 & 0 & -1-\lambda \end{vmatrix}$$

$$=(2-\lambda)(i-\lambda)(-1-\lambda)-(-2)(i-\lambda)$$

$$=(2i-\lambda i-2\lambda+\lambda^2)(-1-\lambda)+2i-2\lambda$$

$$=\cancel{-2i}+\lambda i+\cancel{2\lambda}-\lambda^2-2i\lambda+\lambda^2 i+2\lambda^2-\lambda^3+\cancel{2i}-\cancel{2\lambda}$$

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

$\lambda_1=0$, $\lambda_2=1$, $\lambda_3=i$

are the eigenvalues.

But we know that $\hat{\boldsymbol{M}}\boldsymbol{a}=\lambda\,\boldsymbol{a}$

Eigenvalues and Eigenvectors

But we know that $\hat{M}\boldsymbol{a} = \lambda\,\boldsymbol{a}$

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \lambda_n \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

$$\underbrace{\hat{M}}\qquad a = \lambda\ a$$

Eigenvalues and Eigenvectors

For $\lambda_1 = 0$

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0 \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

This will give 3 equations

$$\begin{cases} 2a_1 - 2a_3 = 0 \\ -2ia_1 + ia_2 + 2ia_3 = 0 \\ a_1 - a_3 = 0 \end{cases}$$

$\longrightarrow a_1 = a_3$

$\Rightarrow a_2 = 0$

Eigenvalues and Eigenvectors

$$\begin{cases} 2a_1 - 2a_3 = 0 & \longrightarrow a_1 = a_3 \\ -2i\,a_1 + i\,a_2 + 2i\,a_3 = 0 & \Rightarrow a_2 = 0 \\ a_1 - a_3 = 0 \end{cases}$$

Imposing $a_1 = 1$ then $\bar{a}_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$ for $\lambda_1 = 0$

Eigenvalues and Eigenvectors

For $\lambda_2 = 1$

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 1\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

This will give 3 equations

$$\begin{cases} 2a_1 - 2a_3 = a_1 \\ -2ia_1 + ia_2 + 2ia_3 = a_2 \\ a_1 - a_3 = a_3 \end{cases}$$

$2a_1 - 2a_3 = a_1 \rightarrow a_3 = \frac{1}{2}a_1$

$\Rightarrow a_2 = \frac{1-i}{2}a_1$

Eigenvalues and Eigenvectors

This will give 3 equations

$$\begin{cases} 2a_1 - 2a_3 = a_1 \\ -2ia_1 + ia_2 + 2ia_3 = a_2 \\ a_1 - a_3 = a_3 \end{cases}$$

$\longrightarrow a_3 = \frac{1}{2} a_1$

$\Rightarrow a_2 = \frac{1-i}{2} a_1$

If $a_1 = 2$ $\quad \bar{a}_2 = \begin{pmatrix} 2 \\ 1-i \\ 1 \end{pmatrix}$ for $\lambda_2 = 1$

Eigenvalues and Eigenvectors

For $\lambda_3 = i$ we have 3 equations

$$\begin{cases} 2a_1 - 2a_3 = ia_1 \\ -2ia_1 + ia_2 + 2ia_3 = ia_2 \\ a_1 - a_3 = ia_3 \end{cases} \Rightarrow a_1 = a_3$$

$a_1 = a_3 = 0$

a_2 is underdetermined so let's put $a_2 = 1$

Eigenvalues and Eigenvectors

a_2 is underdetermined so let's put $a_2 = 1$

$a_1 = a_3 = 0$

$$\bar{a}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \text{for } \lambda_3 = i$$

Eigenvalues and Eigenvectors

$$\hat{T}|\alpha\rangle = \lambda_\alpha|\alpha\rangle$$

- If several eigenvectors correspond to the same eigenvalue, the respective eigenvalue is naturally called "**degenerate**"
- To distinguish between different eigenvectors belonging to the same eigenvalue, I need an additional index

$$\hat{T}\,|\lambda,\mu_n\rangle = \lambda\,|\lambda,\mu_n\rangle$$

λ is n-fold degenerate

Any linear combination of these vectors is again an eigenvector belonging to the same eigenvalue

In fact, if $$|\alpha\rangle = a_1\,|\lambda,\mu_1\rangle + a_2|\lambda,\mu_2\rangle$$

Then $$\hat{T}\,|\alpha\rangle = \hat{T}(a_1\,|\lambda,\mu_1\rangle + a_2|\lambda,\mu_2\rangle) = a_1\,\lambda|\lambda,\mu_1\rangle + a_2\,\lambda|\lambda,\mu_2\rangle = \lambda\,|\alpha\rangle$$

Eigenvalues and Eigenvectors (Theorem)

- Consider two operators commuting operators T and S. Also assume that λ_T is a non-degenerate eigenvalue of T with eigenvector $|\mu_T\rangle$. Then, this vector is also an eigenvector of the operator S.

$$\text{if} \quad \hat{T}\hat{S} = \hat{S}\hat{T} \quad \text{and } \hat{T}|\mu_T\rangle = \lambda_T\,|\mu_T\rangle \text{ then} \quad \hat{S}|\mu_T\rangle = \lambda_S\,|\mu_T\rangle$$

Proof:

$$\hat{S}\hat{T}|\mu_T\rangle = \hat{S}\lambda_T\,|\mu_T\rangle = \lambda_T\hat{S}|\mu_T\rangle$$
$$\hat{T}\hat{S}|\mu_T\rangle = \lambda_T\hat{S}|\mu_T\rangle$$

So $\hat{S}|\mu_T\rangle$ is also an eigenvector of T with still the same eigenvalue λ_T

But we imposed that λ_T is nondegenerate, so $\hat{S}|\mu_T\rangle$ may differ from the initial $|\mu_T\rangle$ only for a constant:

$$\hat{S}|\mu_T\rangle = \lambda_S|\mu_T\rangle$$

thus $|\mu_T\rangle$ is also an eigenvector of S.

- The non-degenerate nature of the eigenvalue of *T* is essential here. But it can be also proved that one can always form such a linear combination of these degenerate eigenvectors which will become an eigenvector of S

Hermitian Operators and Observables

- If you think a bit about Operators, eigenvalues and eigenvectors and all the prosperities that we have discussed, you may find several similarities with Observables, Values of observables and quantum states.

- In fact, the connection is established by some postulates:

1. “Every observable is represented in quantum theory by a Hermitian operator”

2. “If an operator is created to represent an observable, its eigenvalues indicate possible values of a measurement of that observable, and the eigenstates define the quantum state of the system”

Why the operator should be Hermitian? This is due to several properties of the Hermitian Operators...

Hermitian Operators (properties)

- The eigenvalues of Hermitian operators are real

Proof.

Assume that λ is an eigenvalue of T with eigenvector $|\mu\rangle$:

$\hat{T}|\mu\rangle = \lambda|\mu\rangle$.

If I multiply everything by $\langle\mu|$ then:

$$\langle\mu|\hat{T}|\mu\rangle = \langle\mu|\lambda|\mu\rangle = \lambda\langle\mu|\mu\rangle$$

Expectation value (it's a real number)

$*$

$$\langle\mu|\hat{T}^\dagger|\mu\rangle = \lambda^*\langle\mu|\mu\rangle$$

Hermitian Operators (properties)

Proof.

$$\langle \mu | \hat{T} | \mu \rangle = \langle \mu | \lambda | \mu \rangle = \lambda \langle \mu | \mu \rangle$$

Expectation value (it's a real number)

$$*\quad \langle \mu | \hat{T}^{\dagger} | \mu \rangle = \lambda^{*} \langle \mu | \mu \rangle$$

But $\hat{T}^{\dagger} = \hat{T}$ because Hermitian and I can write

$$\hat{T}^{\dagger} | \mu \rangle = \hat{T} | \mu \rangle = \lambda | \mu \rangle$$

so $\lambda \langle \mu | \mu \rangle = \lambda^{*} \langle \mu | \mu \rangle \Rightarrow \lambda = \lambda^{*} \Rightarrow$ real

Hermitian Operators (properties)

Proof.

$$\langle \mu | \hat{T} | \mu \rangle = \langle \mu | \lambda | \mu \rangle = \lambda \langle \mu | \mu \rangle \quad \sigma$$

Expectation value (it's a real number)

λ real, $\langle \mu | \mu \rangle$ = norm of $|\mu\rangle \Rightarrow$ real

Exp. value is real

so $\lambda \langle \mu | \mu \rangle = \lambda^* \langle \mu | \mu \rangle \Rightarrow \lambda = \lambda^* \Rightarrow$ real

Hermitian Operators (properties)

- The eigenvectors of a Hermitian operator belonging to distinct eigenvalues are orthogonal.

Hermitian Operators (properties)

- The eigenvectors of a Hermitian operator belonging to distinct eigenvalues are orthogonal.

Proof.

Assume that λ_1 and λ_2 are two different eigenvalues:

$$\hat{T}|\mu_1\rangle = \lambda_1|\mu_1\rangle \quad \text{and} \quad \hat{T}|\mu_2\rangle = \lambda_2|\mu_2\rangle$$

If I multiply everything by $\langle\mu_2|$ the first one and $\langle\mu_1|$ the second one, then:

$$\langle\mu_2|\hat{T}|\mu_1\rangle = \lambda_1\langle\mu_2|\mu_1\rangle$$

$$\langle\mu_1|\hat{T}|\mu_2\rangle = \lambda_2\langle\mu_1|\mu_2\rangle$$

Hermitian Operators (properties)

Proof.

$$\langle \mu_2 | \hat{T} | \mu_1 \rangle = \lambda_1 \langle \mu_2 | \mu_1 \rangle$$

$$\langle \mu_1 | \hat{T} | \mu_2 \rangle = \lambda_2 \langle \mu_1 | \mu_2 \rangle$$

$*$

$$\langle \mu_2 | \hat{T}^\dagger | \mu_1 \rangle = \lambda_2^* \langle \mu_2 | \mu_1 \rangle$$

$$\hat{T}^\dagger = \hat{T}$$

$$\langle \mu_2 | \hat{T} | \mu_1 \rangle = \lambda_1 \langle \mu_2 | \mu_1 \rangle$$

$$\langle \mu_2 | \underbrace{\hat{T} | \mu_1 \rangle}_{=\lambda_1 | \mu_1 \rangle} = \lambda_2^* \langle \mu_2 | \mu_1 \rangle$$

$$\lambda_2 = \lambda_2^*$$

$$\lambda_1 \langle \mu_2 | \mu_1 \rangle = \lambda_1 \langle \mu_2 | \mu_1 \rangle$$

$$\lambda_1 \langle \mu_2 | \mu_1 \rangle = \lambda_2 \langle \mu_2 | \mu_1 \rangle$$

Hermitian Operators (properties)

Proof.

$$\langle u_2|\hat{T}|u_1\rangle = \lambda_1 \langle u_2|u_1\rangle$$

$$\langle u_1|\hat{T}|u_2\rangle = \lambda_2 \langle u_1|u_2\rangle$$

$$\Rightarrow \lambda_1 \langle u_2|u_1\rangle = \lambda_2 \langle u_2|u_1\rangle$$

but $\lambda_1 \neq \lambda_2$ by hypot.

$$\Rightarrow \langle u_2|u_1\rangle = 0$$

Hermitian Operators (properties)

- The eigenvectors of a Hermitian operator belonging to distinct eigenvalues are orthogonal.

Proof.

Assume that λ_1 and λ_2 are two different eigenvalues:

$$\hat{T}|\mu_1\rangle = \lambda_1|\mu_1\rangle \quad \text{and} \quad \hat{T}|\mu_2\rangle = \lambda_2|\mu_2\rangle$$

Then:

$$\langle\mu_2|\mu_1\rangle = 0 \qquad \text{QED}$$

THE EIGENVECTRORS OF HERMITIAN OPERERATORS ARE ORTHOGONAL

We do see the link between the concept of mutually exclusive states and orthogonal states, being eigenvectors of Hermitian operators.

Hermitian Operators (properties)

- The eigenvectors of a Hermitian Operator span the space, or in other words the collection of Eigenvectors of Hermitian Operators form a complete basis in the Hilbert vector space, still other words, any state in the respective Hilbert space may be represented by a linear combination of the Eigenvectors.

In fact, if we consider a generic state $|\alpha\rangle$:

$$|\alpha\rangle = a_1|q_1\rangle + a_2|q_2\rangle + a_3|q_3\rangle + \cdots = \sum_{i=1}^{N} a_i\,|q_i\rangle$$

Now, q_i are the eigenvectors here.

Remember that $a_1 = \langle q_1|\alpha\rangle$

Then $|\alpha\rangle = \sum_{i=1}^{N} |q_i\rangle\langle q_i|\alpha\rangle = (|q_i\rangle\langle q_i|)\,\alpha\rangle$

Hermitian Operators (properties)

Then $|\alpha\rangle = \sum_{i=1}^{N} |q_i\rangle\langle q_i|\alpha\rangle = \sum_{i=1}^{N} (|q_i\rangle\langle q_i|)\, |\alpha\rangle$

Projector operator $\hat{P}^{(i)}|\alpha\rangle = |q_i\rangle\langle q_i|\alpha\rangle$

And one can easily demonstrate that $\sum_{i=1}^{N} |q_i\rangle\langle q_i| = \hat{I}$

Indeed, proving that $\sum_{i=1}^{N} a_i\, |q_i\rangle = |\alpha\rangle$

In fact:

$a_1 = \langle q_1|\alpha\rangle$ $\quad \sum_{i=1}^{N} a_i\, |q_i\rangle = \sum_{i=1}^{N} |q_i\rangle a_i = \sum_{i=1}^{N} |q_i\rangle\langle q_i|\alpha\rangle = |\alpha\rangle$

Hermitian Operators (properties)

- Then $|\Psi\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\Psi\rangle$

Projector operator $\hat{P}^{(i)}|\Psi\rangle = |\psi_n\rangle\langle\psi_n|\Psi\rangle$

And one can easily demonstrate that $\sum_n |\psi_n\rangle\langle\psi_n| = \hat{I}$

Indeed, proving that $\sum_n c_n |\psi_n\rangle = |\Psi\rangle$