Formalism

Formalism of QM is based on

ψ wave functions

(don't measure ψ; $|\psi|^2$ - prob dens)

represented by (state of a system)

operators

(don't measure operators in the lab - access to expectation values)

represented by (observables)

mathematically: VECTORS ... MATRICES

Operators act on the vectors as linear transformations

language of QM is linear algebra

VECTORS

- real space $\vec{r} = 2\hat{\imath} + 3\hat{\jmath}$, where $\hat{\imath}$ and $\hat{\jmath}$ $\rightarrow$ ORTHONORMAL BASIS

  using the notation $\hat{\imath} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\hat{\jmath} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

  $\vec{r} = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$

→ components are real numbers

→ up to 3D

VECTORS in QM
- $\rightarrow$) complex numbers
- $\rightarrow$) no restriction for dimensions

$$\Psi = |\alpha\rangle$$

$\hookrightarrow$ Ket (Dirac notation)

$$|\alpha\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \vdots \end{pmatrix}$$

$\alpha_1, \alpha_2, \alpha_3, \ldots$ components of $|\alpha\rangle$ in a certain ORTHONORMAL basis

Example
1000 $\rightarrow |\phi_1\rangle$
0100 $\rightarrow |\phi_2\rangle$
0010 $\rightarrow |\phi_3\rangle$
0001 $\rightarrow |\phi_4\rangle$

$$|\alpha\rangle = \alpha_1|\phi_1\rangle + \alpha_2|\phi_2\rangle + \alpha_3|\phi_3\rangle + \alpha_4|\phi_4\rangle$$

orthonormal $\underbrace{(1\,0\,0\,0)}_{\phi_1} \cdot \underbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}}_{\phi_2} = 0$

$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ etc $\qquad |\alpha\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix}$

$\rightarrow$) Vector space: set of vectors with a set of scalars which is CLOSED [= operations are well defined, don't carry you out of the vector space]

under two operations:

- vector addition $\quad |\alpha\rangle + |\beta\rangle = |\gamma\rangle$

  commutative: $|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$

  associative: $|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle$

  zero vector $\quad |\alpha\rangle + |0\rangle = |\alpha\rangle$

  inverse vector $\quad -|\alpha\rangle \Rightarrow |\alpha\rangle + (-|\alpha\rangle) = |0\rangle$

- scalar multiplication $\quad a|\alpha\rangle = |\gamma\rangle$

  distributive, associative

→) linear combinations

$$a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle + \dots = |\Omega\rangle$$

$$\Psi(x) = \sum c_n \psi_n(x)$$

→) linearly independent

$|\lambda\rangle$ is L.I. of $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$ if it cannot be written as a linear comb. of them

Ex: $\hat{k}$ is L.I. of $\hat{\imath}$ and $\hat{\jmath}$ { any vector in xy plane is L. Dependent on $\hat{\imath}$ and $\hat{\jmath}$

→) SPAN

a set of vectors is said to SPAN the space if every vector can be written as a linear combination of this set } set also called COMPLETE

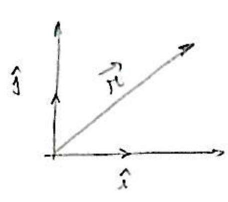
Ex: in 2D $\hat{\imath}$ and $\hat{\jmath}$ SPAN the space

→) BASIS

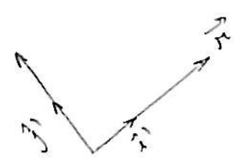
a set of L.I. vectors that SPAN the space { the number of vectors in any basis is the DIMENSION of the space

→) COMPONENTS

in a certain basis, any vector is uniquely represented by its components



$\vec{r} = 2\hat{\imath} + 3\hat{\jmath}$

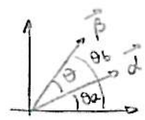


$\vec{r} = \sqrt{13}\ \hat{\imath}'$

the vector is always the same
but its components change according to the basis

→ Inner product

(dot product: $\vec{\alpha}\cdot\vec{\beta} = \alpha\beta\cos\theta$



decomposed in an orthonormal basis $\hat{\imath}, \hat{\jmath}$ $\begin{cases} \hat{\imath}\cdot\hat{\jmath} = 0 \\ \|\hat{\imath}\| = 1 \\ \|\hat{\jmath}\| = 1 \end{cases}$

$$\vec{\alpha}\cdot\vec{\beta} = \alpha\beta\cos\theta = \alpha\beta\cos(\theta_b - \theta_a) = \alpha\beta\,(\cos\theta_b\cos\theta_a + \sin\theta_b\sin\theta_a)$$

$$= \alpha\beta\left(\frac{b_x\, a_x}{\alpha\beta} + \frac{b_y\, a_y}{\alpha\beta}\right) = a_x b_x + a_y b_y$$

$$\vec{\alpha}\cdot\vec{\beta} = \underbrace{(a_x \quad a_y)}_{\substack{\text{row} \\ \text{vector} \\ \langle\alpha|}} \underbrace{\begin{pmatrix} b_x \\ b_y \end{pmatrix}}_{\substack{\text{colum vector} \\ |\beta\rangle}} = \langle\alpha|\beta\rangle = a_x b_x + a_y b_y \quad)$$

$\langle\alpha|\beta\rangle$

$$|\beta\rangle = \overbrace{b_1 \ldots b_2 \ldots b_3}^{\text{COMPONENTS}} \quad |\beta\rangle = b_1|e_1\rangle + b_2|e_2\rangle + b_3|e_3\rangle + \ldots$$

BASIS

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + a_3|e_3\rangle + \ldots$$

$$\Longrightarrow \langle\alpha| = \langle e_1|\, a_1^* + \langle e_2|\, a_2^* + \langle e_3|\, a_3^* + \ldots$$

bra

bracket

$$\langle\alpha|\beta\rangle = a_1^* b_1 \langle e_1|e_1\rangle + a_1^* b_2 \langle e_1|e_2\rangle + a_1^* b_3 \langle e_1|e_3\rangle + \ldots$$

BUT, if the basis is ORTHONORMAL ⟷ $\boxed{\langle e_i|e_j\rangle = \delta_{ij}}$

then

$$\boxed{\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + a_3^* b_3 + \ldots}$$ ⟵ very convenient

$$\hookrightarrow \underbrace{(a_1^* \quad a_2^* \quad a_3^* \ldots)}_{\text{(row vector)}} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix} \text{(column vector)}$$ } because basis is orthonormal

most of the vectors we encounter in QM are functions and they live in

infinite – dimensional spaces

The collection of all functions of x constitutes a vector space

But to represent a possible physical state it must be normalized

$$\int |\psi|^2 dx = 1$$

→) The set of all square-integrable functions on an interval

$f(x)$ such that $\int_a^b |f(x)|^2 dx < \infty$

constitutes a vector space called

$$\boxed{\text{HILBERT SPACE}}$$

In a infinite dim space, we define the inner-product as

$$\boxed{\langle f|g\rangle \equiv \int_a^b f(x)^* g(x)\, dx}$$

Properties:

- $\langle g|f\rangle = \langle f|g\rangle^*$
- $\langle f|f\rangle \geq 0$
- NORM: $\|f\| \equiv \sqrt{\langle f|f\rangle}$
- If $\|f\| = 1$ → vector / function is normalized

  Ex: $\|\alpha\| = \sqrt{\langle\alpha|\alpha\rangle} = 1 \Rightarrow \boxed{|a_1|^2 + |a_2|^2 + |a_3|^2 + \dots = 1}$
- $\langle f|g\rangle = 0$ ← orthogonal ; $\langle f_m|f_n\rangle = \delta_{mn}$ ← orthonormal
- set is complete if any function (in Hilbert space) can be expressed as linear comb

  $f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$ (orthonorm.) $\boxed{c_n = \langle f_n|f\rangle}$

MATRICES $\longrightarrow$ operators

multiply vectors by a scalar
rotate vectors

linear transformations T

$$\hat{T}|\alpha\rangle = |\alpha'\rangle$$

◦) transpose $\tilde{T}$

symmetric: $T = \tilde{T}$ antisym: $\tilde{T} = -T$

◦) complex conjugate T^*

real: $T^* = T$ imagin: $T^* = -T$

$\Rightarrow$) hermitian conjugate (or ADJOINT)

$$\boxed{T^\dagger = \tilde{T}^*}$$

square matrix is hermitian (or self-adjoint) if it is equal to $T^\dagger$

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

$$(|\alpha\rangle)^\dagger = \langle\alpha|$$

bra is the hermitian conjugate of the ket (and vice-versa)

OBSERVABLES are represented by hermitian operators

$$\begin{cases} \langle w|v\rangle \overset{|v\rangle = T|u\rangle}{=} \langle w|T|u\rangle \\ \langle w|v\rangle^* = \langle v|w\rangle \underset{\langle v| = \langle u|T^\dagger}{=} \langle u|T^\dagger|w\rangle \end{cases}$$

Expectation value of an OBSERVABLE

$$\langle T\rangle = \int \psi^* \hat{T}\, \psi\, dx = \langle \psi | T | \psi \rangle$$

$$\langle T\rangle = \overset{\langle\psi|T\psi\rangle}{\langle \psi | T | \psi \rangle}$$

(see next page)

$$\langle \psi | T\psi\rangle^* = \langle T\psi | \psi\rangle \overset{\downarrow}{=} \langle \psi | T^\dagger | \psi\rangle$$

$$\langle T\rangle^* = \left(\langle \psi | T | \psi\rangle\right)^* = \langle \psi | T^\dagger | \psi\rangle$$

since the outcome of a measurement has to be real

$$\Downarrow$$

$$\langle T\rangle = \langle T\rangle^*$$

$$\Downarrow$$

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

a square matrix T is hermitian (or self-adjoint) if it is equal to $T^\dagger$

OBSERVABLES are represented by hermitian operators

Is momentum a hermitian operator?

$$\langle p\rangle = \langle \psi | p | \psi\rangle = \int \psi^* \frac{\hbar}{i} \frac{d\psi}{dx}\, dx$$

$$\langle p\rangle^* = \langle \psi | p | \psi\rangle^* = \int \left(\psi^* \frac{\hbar}{i}\frac{d\psi}{dx}\right)^* dx = \int \psi \left(-\frac{\hbar}{i}\frac{d\psi^*}{dx}\right) dx$$

by parts $\cancel{-\frac{\hbar}{i}\psi\psi^*\Big|_{-\infty}^{\infty}} + \frac{\hbar}{i}\int \frac{d\psi}{dx}\psi^*\, dx = \int \psi^* \frac{\hbar}{i}\frac{d\psi}{dx}\, dx$

or $\langle p\rangle - \langle p\rangle^* = \int \frac{\hbar}{i}\frac{d}{dx}(\psi^*\psi)\, dx = \frac{\hbar}{i}\psi^*\psi\Big|_{-\infty}^{\infty} = 0$

$$\Rightarrow \langle p\rangle = \langle p\rangle^* \Rightarrow \boxed{\hat{p} = \hat{p}^\dagger}$$

more generally, a hermitian operator satisfies

$$\boxed{\langle \psi_1 | T\psi_2 \rangle = \langle T\psi_1 | \psi_2 \rangle}$$

which is equivalent to

$$\boxed{T = T^+}$$

because

$$\langle T\psi_1 | \psi_2 \rangle = \langle \psi_1 | T^+ | \psi_2 \rangle$$

Showing that

$$\langle T\psi_1 | \psi_2 \rangle = \langle \psi_1 | T^+ | \psi_2 \rangle$$

with matrices

$$|T\psi_1\rangle = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \overbrace{\begin{pmatrix} t_{11} a_1 + t_{12} a_2 \\ t_{21} a_1 + t_{22} a_2 \end{pmatrix}}^{\text{column}} \Rightarrow \langle T\psi_1 | = \left(|T\psi_1\rangle \right)^+ = \overbrace{\begin{pmatrix} t_{11}^* a_1^* + t_{12}^* a_2^* & t_{21}^* a_1^* + t_{22}^* a_2^* \end{pmatrix}}^{\text{row}}$$

$$\langle \psi_1 | T^+ = \begin{pmatrix} a_1^* & a_2^* \end{pmatrix} \begin{pmatrix} t_{11}^* & t_{21}^* \\ t_{12}^* & t_{22}^* \end{pmatrix} = \begin{pmatrix} a_1^* t_{11}^* + a_2^* t_{12}^* & a_1^* t_{21}^* + a_2^* t_{22}^* \end{pmatrix} \leftarrow (=)$$

$$\Downarrow$$

$$\boxed{\langle T\psi_1 | = \langle \psi_1 | T^+}$$

Showing that momentum is a hermitian operator

$$\langle f | pg \rangle = \int f^* \frac{\hbar}{i} \frac{dg}{dx}\, dx = \cancel{\frac{\hbar}{i} f^* g \Big|_{-\infty}^{\infty}} - \frac{\hbar}{i} \int \frac{df^*}{dx}\, g\, dx = \int \left(\frac{\hbar}{i} \frac{d f}{dx} \right)^* g\, dx$$

$$= \boxed{\langle pf | g \rangle}$$

•) matrix multiplication is not, in general, commutative

commutator: $[S,T] = ST - TS$

•) transpose of product is transpose of each in reverse order

$$\widetilde{(ST)} = \tilde{T}\tilde{S}$$

$$\widetilde{(ST)}_{ki} = (ST)_{ik} = \sum_j S_{ij} T_{jk} = \sum_j T_{jk} S_{ij} = \sum_j (\tilde{T})_{kj} (\tilde{S})_{ji} = (\tilde{T}\tilde{S})_{ki}$$

$$\underbrace{A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad \tilde{A} = \begin{pmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{pmatrix}}$$

$$A_{12} = \tilde{A}_{21}$$

$$a_{12} = a_{12}$$

$$\Rightarrow \widetilde{(ST)} = \tilde{T}\tilde{S}$$

•) hermitian conjugate

$$(ST)^{+} = T^{+} S^{+}$$

$$(ST)^{+} = \widetilde{(ST)}^{*} = (\tilde{T}\tilde{S})^{*} = T^{+} S^{+}$$

•) unit matrix $\quad \mathbb{1} = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & 1 \ddots \end{pmatrix}$

o) inverse of a square matrix

$$T^{-1}\,T = T\,T^{-1} = \mathbb{1}$$

$$\boxed{T^{-1} = \frac{1}{\det T}\,\tilde{C}}$$

transpose matrix of cofactors

$C_{11} = d(-1)^2 \quad C_{12} = c(-1)^3$
$C_{21} = b(-1)^3 \quad C_{22} = a(-1)^4$
$\Rightarrow \tilde{C} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow \det A = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = \boxed{ad - bc}$$

$$\boxed{A^{-1} = \frac{1}{(ad-bc)}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}}$$

$$A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \Rightarrow \det A = \underbrace{a\begin{vmatrix} e & f \\ h & i \end{vmatrix}}_{C_{11} = a(-1)^{1+1}|\;|} \underbrace{- b\begin{vmatrix} d & f \\ g & i \end{vmatrix}}_{C_{12} = b(-1)^{1+2}|\;|} \underbrace{+ c\begin{vmatrix} d & e \\ g & h \end{vmatrix}}_{C_{13} = c(-1)^{1+3}|\;|}$$

cofactors for one row or one column

cofactor $C_{ij} = (-1)^{i+j}\underbrace{|M_{ij}|}_{}$

$(n-1)\times(n-1)$ matrix that results from deleting i-th row and j-th column of original matrix

⇒) unitary matrix

$$\boxed{U^{\dagger} = U^{-1}}$$

evolution operator of a CLOSED syst is unitary