Formalism

Formalism of QM is based on

- **Wave functions**
  - | don't measure | (do measure)
  - | don't change probability | (state of a system)

- **Operators**
  - | don't measure operators | (operators in the lab - access to expectation values)
  - | observables | (observables)

Mathematically:

- **Vectors**
- **Matrices**

Operators act on the vectors as linear transformations.

Language of QM in linear algebra

**VECTORS**

1) Real space: \[ \vec{r} = 2\hat{i} + 3\hat{j} \]

Using the notation:

\[ \hat{i} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \hat{j} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \]

\[ \vec{r} = \begin{pmatrix} 2 \\ 3 \end{pmatrix} \]

- Components are real numbers.
- Up to 3D
VECTORS in QM

1) complex numbers
2) no restriction for dimension

\[ \Psi = 1d> \]

\( 1d> = \begin{pmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{pmatrix} \)

- components of \( 1d> \) in an orthonormal basis

Example:

\[ 1d> = d_1 1\beta> + d_2 1\gamma> + d_3 1\delta> + d_4 1\theta> \]

\[ |\beta> = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \]

\[ |\gamma> = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \]

\[ |\delta> = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \]

\[ |\theta> = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \]

Vector space - set of vectors with a set of scalars which is closed [op-n-sions are well-defined; don't carry you out of the vector space]

under two operations:

1) vector addition \( 1d> + |\beta> = 1\beta> \)

- commutative
- associative

\[ 1d> + |\beta> = |\beta> + 1d> \]

- inverse \( \iota d> = 1d> \)

2) scalar multiplication \( a |d> = |\alpha d> \)

- distributive, associative
\( \text{linear combination} \)

\[ a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle + \ldots = |\Omega\rangle \]

\[ \Psi(x) = \Sigma c_n \Psi_n(x) \]

\( \rightarrow \) \text{linearly independent}

\( |\Omega\rangle \text{ is L.I. of } |\alpha\rangle, |\beta\rangle, |\gamma\rangle \text{ if it cannot be written as a linear comb of them} \)

\( \text{Ex: } \vec{e} \text{ in L.I. of } \vec{x} \text{ and } \vec{y} \text{ any vector in xy plane is L. Dependent on } \vec{x} \text{ and } \vec{y} \)

\( \rightarrow \) \text{SPAN}

\( \text{a set of vectors is said to span the space if every vector can be written as a linear combination of this set} \)

\( \text{Ex: in 2D } \vec{x} \text{ and } \vec{y} \text{ span the space} \)

\( \rightarrow \) \text{BASIS}

\( \text{a set of L.I. vectors that span the space} \)

\( \rightarrow \) \text{COMPONENTS}

\( \text{in a certain basis, any vector is uniquely represented by its components} \)

\[ \vec{A} = \theta \hat{i} + \theta \hat{j} \]

\( \vec{r} = \sqrt{13} \hat{x} \)

\( \text{the vector is always the same but its components change according to the basis} \)
Inner product

\[ \langle d | \beta \rangle = d \beta \] where \( d \beta \) is decomposed in an orthonormal basis \( e_i \):

\[ d \beta = d \beta_{e_1} e_1 + d \beta_{e_2} e_2 + d \beta_{e_3} e_3 + \cdots \]

\[ \langle d | \beta \rangle = \begin{pmatrix} a_x \\ a_y \end{pmatrix} \begin{pmatrix} b_x \\ b_y \end{pmatrix} = \langle d | \beta \rangle = \langle x | b \rangle = ax b_x + ay b_y \]

\[ \langle d | \beta \rangle = \begin{pmatrix} a_x \\ a_y \end{pmatrix} \begin{pmatrix} b_x \\ b_y \end{pmatrix} = \langle d | \beta \rangle = \begin{pmatrix} b_1 a_x \\ b_2 a_x \end{pmatrix} + \begin{pmatrix} b_1 a_y \\ b_2 a_y \end{pmatrix} + \begin{pmatrix} b_3 a_x \\ b_3 a_y \end{pmatrix} + \cdots \]

**Basis**

**Components**

Then

\[ \langle d | \beta \rangle = c_1 e_1 + c_2 e_2 + c_3 e_3 + \cdots \]

**But, if the basis is ORTHONORMAL**

**very convenient**

\[ \langle d | \beta \rangle = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \]

because basis is orthonormal
most of the vectors we encounter in QM are functions
and they live in

\textit{infinite-dimensional space}

the collection of all functions of x constitutes a vector space
But to represent a physical state it must be normalized

\[ \int |\psi|^2 \, dx = 1 \]

2) The set of all square-integrable functions on an interval
\[ f(x) \text{ such that } \int_0^b |f(x)|^2 \, dx < \infty \]
forms a vector space called

\textit{Hilbert Space}

In an infinite dim space, we define the inner product as

\[ \langle f | g \rangle = \int_a^b f(x)^* g(x) \, dx \]

\textbf{Properties:}

0) \[ \langle f | f \rangle = \langle f | g \rangle^* \]
1) \[ \langle f | f \rangle \geq 0 \]
2) \textit{Norm:} \[ \|f\| \equiv \langle f | f \rangle \]
3) If \( \|f\| = 1 \rightarrow \text{vector/function is normalized} \]
   \[ \text{Ex. } \|f\|^2 = \int f(x)^2 \, dx = 1 \Rightarrow 101^2 + 102^2 + 103^2 + \ldots = 1 \]
4) \( \langle f | g \rangle = 0 \rightarrow \text{orthogonal} ; \langle f_m | f_n \rangle = \delta_{mn} \rightarrow \text{orthonormal} \]
5) \textit{set is complete if any function (in Hilbert space) can be expressed as linear combo}
   \[ f(x) = \sum c_n f_n(x) \quad \text{(orthonormal)} \quad \|c_n\| = \langle f_n | f \rangle \]
**MATRICES** → **operations**

- multiply vectors by a scalar
- rotate vectors

**linear transformations (T)**

\[ T \hat{1} = \hat{1} \hat{v} \]

1) **transpose (T)**

- symmetric: \( T = T^\dagger \)
- anti-symmetric: \( T = -T \)

2) **complex conjugate (\( T^\dagger \)**)

- real: \( T^\dagger = T \)
- imaginary: \( T^\dagger = -T \)

3) **Hermitian conjugate (or adjoint)**

\[ T^\dagger = T^\ast \]

\[ (1 \hat{v})^\dagger = \hat{v}^\dagger \]

Bra is the hermitian conjugate of the ket (and vice versa)

**Observables are represented by Hermitian operators**

\[
\begin{align*}
\langle \omega | T | \omega \rangle &= \langle \omega | T^\ast | \omega \rangle \\
\langle \omega | \omega \rangle &= \langle \omega | T^\dagger | \omega \rangle \\
\omega | \omega \rangle &= \langle \omega | T^\dagger | \omega \rangle
\end{align*}
\]

\[ \omega | \omega \rangle = \langle \omega | T^\dagger | \omega \rangle \]
Expectation value of an observable

\[ \langle T \rangle = \int \psi^* T \psi \, dx = \langle \psi | T | \psi \rangle \]

\[ \langle \psi | T | \psi \rangle \]

\[ \langle \psi | T | \psi \rangle = \langle T \psi | \psi \rangle = \langle \psi | T \psi \rangle \]

\[ \langle T \rangle = \left( \langle \psi | T | \psi \rangle \right)^* = \langle T^* \psi | \psi \rangle \]

\[ \langle T \rangle = \langle T^* \rangle \]

\[ \sqrt{T} = T^+ \]

\[ \text{a square matrix is hermitian (or self-adjoint)} \]

\[ \text{if it is equal to } T^+ \]

\[ \{ \text{observables are represented by hermitian operators} \} \]

Is momentum a hermitian operator?

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

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

\[ \text{by parts: } -\frac{\hbar}{i} \psi \frac{d\psi}{dx} \bigg|_0^\infty + \frac{\hbar}{i} \int_0^\infty \frac{d\psi}{dx} \psi \, dx = \int \psi^* \frac{\hbar}{i} \frac{d\psi}{dx} \, dx \]

\[ \text{or } \langle p \rangle = \langle p^* \rangle = \int \frac{\hbar}{i} \frac{d}{dx} (\psi \psi^*) \, dx = \frac{\hbar}{i} \psi \psi^* \bigg|_0^\infty = 0 \]

\[ \Rightarrow \langle p \rangle = \langle p^* \rangle \Rightarrow \hat{p} = \hat{p}^+ \]
more generally, a hermitian operator satisfies

\[ \langle \Psi_2 | T \Psi_2 \rangle = \langle T \Psi_2 | \Psi_2 \rangle \]

which is equivalent to

\[ T = T^+ \]

because

\[ \langle T \Psi_2 | \Psi_2 \rangle = \langle \Psi_2 | T^+ \Psi_2 \rangle \]

Showing that

\[ \langle T \Psi_1 | \Psi_1 \rangle = \langle \Psi_1 | T^+ \Psi_1 \rangle \]

with matrices

\[
\begin{pmatrix}
1T \Psi_1 \\
\end{pmatrix}
= 
\begin{pmatrix}
in_1 & l_{12} \\
l_{21} & l_{22}
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2
\end{pmatrix}
= 
\begin{pmatrix}
in_1 a_1 + l_{12} a_2 \\
l_{21} a_1 + l_{22} a_2
\end{pmatrix}
= \langle T \Psi_1 | \rangle = \langle 1T \Psi_1 | \rangle^T = 
\begin{pmatrix}
\text{row} \\
\text{column}
\end{pmatrix}
\begin{pmatrix}
\bar{a}_1 & \bar{a}_2 \\
\bar{a}_2 & \bar{a}_1
\end{pmatrix}
\begin{pmatrix}
\bar{a}_1 \\
\bar{a}_2
\end{pmatrix}
\]

\[ \langle \Psi_2 | T^+ \rangle = \langle \bar{a}_1 \bar{a}_2 \rangle = 
\]

\[ \langle \Psi_1 | T^+ \rangle \]

\[ \langle T \Psi_2 | \rangle = \langle \Psi_1 | T^+ \rangle \]

Showing that momentum is a hermitian operator

\[ \langle f | p \cdot g \rangle = \int f^* \frac{\hbar}{i} \frac{d}{dx} g \ dx = \frac{\hbar}{i} [ f^* \frac{d}{dx} g ] - \frac{\hbar}{i} \int \frac{df^*}{dx} \ g \ dx = \int \left( \frac{\hbar}{i} \frac{df^*}{dx} \right) g \ dx = \]

\[ \langle p \cdot f | g \rangle \]
1) matrix multiplication is not, in general, commutative

\[ [S, T] = ST - TS \]

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

\[ (ST)^T = T^S \]

\[ (ST)^{\prime} = (S^T)^{\prime} = (T^S)^{\prime} = T^S \]

3) unit matrix

\[ \mathbf{I} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \]
0) inverse of a square matrix

\[ T^{-1} T = T T^{-1} = I \]

\[ T^{-1} = \frac{1}{\text{det}(T)} \]

\[ A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow \text{det} A = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc \]

\[ A^{-1} = \frac{1}{\text{det}(A)} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \]

\[ A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \Rightarrow \text{det} A = \begin{vmatrix} a & e & f \\ d & g & h \\ c & d & e \end{vmatrix} \]

\[ C_{ij} = (-1)^{i+j} [M_{ij}] \]

\[ \text{submatrix that results from deleting } i \text{th row and } j \text{th column of original matrix} \]

\[ (n-1) \times (n-1) \text{ matrix for one row or one column} \]

\[ \Rightarrow \text{unitary matrix} \]

\[ U^* = U^{-1} \]

\[ \text{evolution operator of a closed cycle is unitary} \]