Intuitive Introduction to Formalism

Maths as tool so that struggling with Physics is enjoyable.

11.1 Ket vectors live in $\mathcal{H}$

A linear Vector space: $\begin{cases} \text{Vectors and scalars} \\ \text{Vector Addition \& Scalar Multiplication} \end{cases}$

[Commutative, Associative, $\exists$ neutral zero, Inverse]
unit scalar, zero scalar]

$$|\psi\rangle = a|\phi\rangle + b|\chi\rangle$$

Linear combination is also a vector.

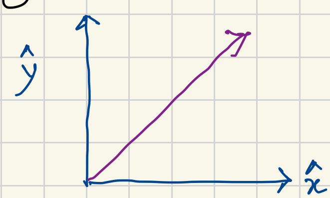
a and b can be complex

If ϕ an χ belong to $\mathcal{H}$ then any linear combination also belong to $\mathcal{H}$

Cauchy Complete

Technically required to keep infinities out of analysis.

Generalization of ordinary Euclidean vectors.



Two orthogonal unit vectors needed to span the space.

However, two orthonormal cannot span 3-dim vector.

We need $(\hat{\imath}, \hat{\jmath}, \hat{k})$ or $(\hat{r}, \hat{\theta}, \hat{\varphi})$ (spherical) or $(\hat{r}, \hat{\varphi}, \hat{z})$ (cylindrical)

- Dimension of Vector Space:

N-dim discrete

$$|\psi\rangle = \sum_{i=1}^{N} c_i |e_i\rangle$$

basis vectors

Examples: - Infinite: $1, \sin x, \sin 2x, \ldots$

- All the solutions of 1-D particle in a box (discrete and infinite)

- Finite: $|\uparrow\rangle$ $|\downarrow\rangle$ 2 basis functions. spin up and spin down for electrons.

The notion of '<u>completeness</u>':

Number of orthogonal basis vectors needed to span all possible vectors in the linear vector space.

A set of such orthonormal vectors is said to be 'complete'.

The set can be finite or infinite
discrete or continuous.

Think of examples from our discussion in previous chapters.

BRA & KET in $\mathcal{H}$ and $\mathcal{H}_d$

- For every ket has a corresponding bra.

$\mathcal{H}$:

$\mathcal{H}_d$: dual Hilbert space.

$$|\psi\rangle \longleftrightarrow \langle\psi|$$

$$a|\psi\rangle + b|\phi\rangle \longleftrightarrow a^*\langle\psi| + b^*\langle\phi|$$

$$|a\psi\rangle = a|\psi\rangle \qquad \langle a\psi| = a^*\langle\psi|$$

- $\langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle$ $\qquad$ $|\psi\rangle^\dagger = \langle\psi|$

- Norm is real and positive.

Suppose we did not have complex conjugation, then norm need not be positive. $\langle ia|ia\rangle = a^2$ because of conjugation.

The necessity of conjugation in bra.

- Schwarz Inequality :

$$|\langle\phi|\psi\rangle|^2 \leq \langle\phi|\phi\rangle\langle\psi|\psi\rangle$$

Familiar vector relation $|\vec{A}\cdot\vec{B}|^2 \leq |\vec{A}|^2|\vec{B}|^2$

Generalization for functions.

- Triangle Inequality :

$$\sqrt{\langle\psi+\phi|\psi+\phi\rangle} \leq \sqrt{\langle\psi|\psi\rangle} + \sqrt{\langle\phi|\phi\rangle}$$

- Orthogonal / Orthonormal

$$\left.\begin{aligned} &\langle\psi|\phi\rangle = 0 \\ &\langle\psi|\psi\rangle = 1 \quad \langle\phi|\phi\rangle = 1 \end{aligned}\right\}$$

Both conditions satisfied for orthonormality.

L11: 4/10 ynm

- $|\psi\rangle$ as a column vector $\langle\phi|$ as a row vector.

Think of $|\psi\rangle = \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \psi(x_3) \\ \vdots \end{pmatrix}$ and $\langle\phi| = (\phi_1^*, \phi_2^*, \phi_3^*, \cdots)$

$$\langle\phi|\psi\rangle = (\phi_1^*, \phi_2^*, \phi_3^* \cdots) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \end{pmatrix} = \sum_{i=1}^{N} \phi_i^* \psi_i$$

(discrete)

Looks like a dot product with complex co-efficients.

For continuous functions

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

Definition of INNER PRODUCT

Generalized dot product

Inner Product : - Matrix multiplication in finite.

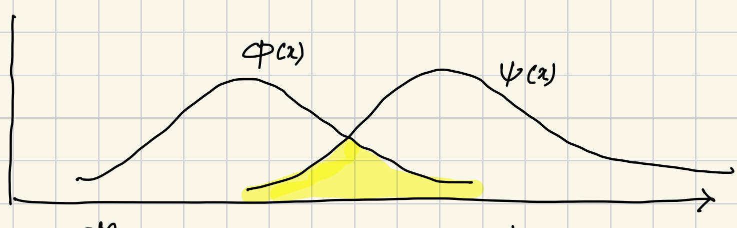
- Angle, Norm.
- Measure of overlap.

These notions generalized.

Example with real functions:

$$\int_{-\infty}^{\infty} \phi^*(x)\,\psi(x)\,dx = 0$$

orthogonal.



How much $|\phi\rangle$ is in $|\psi\rangle$?

$$\langle\phi|\psi\rangle = \int_{-\infty}^{\infty} \phi^*(x)\,\psi(x)\,dx \longleftarrow \text{degree of overlap.}$$

Inner product

Operators: Instructions to act on Kets & Bras.

- $\hat{A}\,|\psi\rangle = |\psi'\rangle$ $\qquad$ $\langle\phi|\vec{A} = \langle\phi'|$

The modified $|\psi'\rangle$ or $\langle\phi'|$ must belong to $\mathcal{H}$ and $\mathcal{H}_d$ respectively.

- Products of Operators
  - $\hat{A}\hat{B} \neq \hat{B}\hat{A}$ $\qquad$ Generally not commutative
  - Order of application is important

    $$\hat{A}\hat{B}\,|\psi\rangle = \hat{A}\left(\hat{B}|\psi\rangle\right)$$

  - $$\langle\varphi|\hat{A}|\psi\rangle \equiv \left(\langle\varphi|\hat{A}\right)|\psi\rangle \equiv \langle\varphi|\left(\hat{A}\psi\right)\rangle$$

    – a complex number.

- Linear Operators:

  $$\hat{A}\left(a_1|\psi_1\rangle + a_2|\psi_2\rangle\right) = a_1\hat{A}|\psi_1\rangle + a_2\hat{A}|\psi_2\rangle$$

- Expectation value wrt $|\psi\rangle$

- $|\phi\rangle\langle\psi|$ is a linear operator

  Proof: $\quad |\phi\rangle\langle\psi||\psi'\rangle = \underbrace{\langle\psi|\psi'\rangle}_{\text{complex no.}}|\phi\rangle$

$\left.\begin{array}{l} |\psi\rangle\hat{A} \\ \hat{A}\langle\psi| \end{array}\right\}$? $\leftarrow$ These have no meaning as such!

Adjoint of $\hat{A}$ (simply adjoint)

$$\boxed{\langle\psi|\hat{A}^\dagger|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*}$$

Definition.

Flip & Conjugate

1. $a^\dagger = a^*$
2. $|\psi\rangle^\dagger = \langle\psi|$
3. $\hat{A} \rightarrow \hat{A}^\dagger$

Try writing the right side

$$(\hat{A}^\dagger)^\dagger =$$

$$(a\hat{A})^\dagger =$$

$$(A+B+C)^\dagger =$$

$$(ABC|\psi\rangle)^\dagger =$$

$$|a\hat{A}\psi\rangle = \qquad \langle a\hat{A}\psi| =$$

$$\langle a\hat{A}^\dagger\psi| = a^*\langle\psi|(\hat{A}^\dagger)^\dagger = a^*\langle\psi|\hat{A}$$

$$\langle\psi|\hat{A}|\phi\rangle = \langle\hat{A}^\dagger\psi|\phi\rangle = \langle\psi|\hat{A}\phi\rangle$$

Adjoint of $\hat{A}$ (simply adjoint)

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Definition.

Flip & Conjugate

1. $a^\dagger = a^*$
2. $|\psi\rangle^\dagger = \langle\psi|$
3. $\hat{A} \to \hat{A}^\dagger$

$$(\hat{A}^\dagger)^\dagger = \hat{A}$$

$$(a\hat{A})^\dagger = a^*\hat{A}^\dagger$$

$$(A+B+C)^\dagger = A^\dagger + B^\dagger + C^\dagger$$

$$(ABC|\psi\rangle)^\dagger = \langle\psi|C^\dagger B^\dagger A^\dagger$$

$$|a\hat{A}\psi\rangle = a\hat{A}|\psi\rangle \qquad \langle a\hat{A}\psi| = a^*\langle\psi|A^\dagger$$

$$\langle a\hat{A}^\dagger\psi| = a^*\langle\psi|(\hat{A}^\dagger)^\dagger = a^*\langle\psi|\hat{A}$$

$$\langle\psi|\hat{A}|\phi\rangle = \langle\hat{A}^\dagger\psi|\phi\rangle = \langle\psi|\hat{A}\phi\rangle$$

You must have encountered adjoint in matrices.
Same idea with complex functions.

To take Adjoint : flip, dagger, * | sequence.

L-11 : 8/10 ynm

Hermitian Operators:

Operators that are self-adjoint.

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

Hermitian Definition

or, $\langle \psi | \hat{A} | \phi \rangle = \langle \phi | \hat{A} | \psi \rangle^*$

Operator remains same on flip and *

Note: In general, $\underbrace{\hat{A}^{\dagger} \neq \hat{A}^*}$

For QM operators not acceptable.

Skew Hermitian:

(also called anti-Hermitian) $\hat{B}^{\dagger} = -\hat{B}$ or $\langle \psi | \hat{B} | \phi \rangle = -\langle \phi | \hat{B} | \psi \rangle^*$

Example:

i) $\int \varphi^* \dfrac{d\psi}{dx}\, dx$ | show that $\dfrac{d}{dx}$ is anti-Hermitian

ii) $-i\hbar \dfrac{d}{dx}$ is Hermitian?

iii) Is $\hat{x}$ Hermitian?

Important Properties of Hermitian $\hat{A}$

Claim: Expectation of Hermitian $\hat{A}$ is real.

$$\langle \psi | \hat{A} | \phi \rangle = \langle \phi | \hat{A} | \psi \rangle^* \qquad \text{Defn:}$$

$$\therefore \quad \langle \psi | \hat{A} | \psi \rangle = \langle \psi | \hat{A} | \psi \rangle^*$$

i.e. If $\hat{A}^\dagger = \hat{A}$ then $\langle \hat{A} \rangle$ is real.

For anti-Hermitian (or, skew Hermitian)

$$\hat{B}^\dagger = -\hat{B} \qquad \text{or,} \quad \langle \psi | \hat{B} | \phi \rangle = -\langle \phi | \hat{B} | \psi \rangle^*$$

- The requirement of Hermiticity in physical operators stems from the need to have their expectation value real.
- All operators corresponding to physical observables must be Hermitian.

L11 : 10/10 ynm

Ex. What is the Adjoint of $\frac{d}{dx}$

$$\left(\frac{d}{dx}\right)^{\dagger} = -\frac{d}{dx}$$

$$\langle f | \tfrac{d}{dx} | g\rangle = \int_{-\infty}^{\infty} f^* \frac{dg}{dx}\, dx$$

Integrating by parts.

$f, g \to 0$ at $-\infty, \infty$

$$= \cancel{f^* g\Big|_{-\infty}^{\infty}}_{0} - \int_{-\infty}^{\infty} \frac{df^*}{dx}\, g\, dx = -\langle f | \tfrac{d}{dx} | g\rangle$$

anti-Hermitian

$$\langle f | \hat{p} | g\rangle = \int_{-\infty}^{\infty} f^* \left(\frac{\hbar}{i}\frac{dg}{dx}\right) dx$$

$$= \frac{\hbar}{i}\cancel{f^* g\Big|_{-\infty}^{\infty}}^{\to 0} - \frac{\hbar}{i}\int_{-\infty}^{\infty} \left(\frac{df}{dx}\right)^* g\, dx$$

$$= \int_{-\infty}^{\infty} \left(\frac{\hbar}{i}\frac{df}{dx}\right)^* g\, dx = \langle \hat{p} f | g\rangle$$ Hermitian

Note the function of i in $\hat{p}$.

Adjoint of $\hat{x}$?

$$\langle f | x g\rangle = \int f^* (x g)\, dx = \int x f^* g\, dx$$

$$= \int (xf)^* g\, dx = \langle xf | g\rangle$$

$$\boxed{x^{\dagger} = x}$$ Hermitian.

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