Vector & Function Spaces

Re-casting our QM Formalism

Using Linear Algebra - Intro due

Hermitian or Self-Adjoint Ops

& role in QM.

We'll start by reviewing what we already knew about

V.S. \( \frac{1}{2} E.S.'s \)
\[ F = F_x \hat{i} + F_y \hat{j} \]

or write:
\[ \vec{F} = (F_x, F_y) \]

\[ \{ \hat{i}, \hat{j} \} = \text{linearly indep basis} \]
That completely "spans" 2-D
\[ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ row reduced echelon from Gaussian elimination} \]

Introduce The dot product = Inner Product in F.S.

\[ \vec{A} \cdot \vec{B} = A_x B_x + A_y B_y \]

\[ \text{Using } \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix} \]

\[ \vec{e}_0 \cdot \vec{e}_0 = \delta_{0,0} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{else} \end{cases} \]

Now it is had \( \infty \) V.S. dot prod would like
\[ A_1 B_1 + A_2 B_2 + A_3 B_3 + \ldots + A_n B_n \]

\[ s(x) = \sum_{n=0}^{\infty} \sin(n \omega x) + \sum_{n=0}^{\infty} \cos(n \omega x) \]

\[ = \text{Fourier Series or:} \]

\[ \int_{-\infty}^{\infty} s(x) e^{i \omega x} \, dx \]

\[ = \text{Fourier Integral} \]

\[ \sin(x) \text{ & } \cos(x) = \text{infty-D} \]
\[ \text{Linearly indep Basis} \]
That completely "fills" all of such space (i.e. WROKSIKIANZ0)

\[ \text{extend to F.S. which is} \]

\[ \text{have not vectors } (\vec{A}, \vec{B}) \]
\[ \text{but functions say } s(x), g(x) \]

So the \( \infty \) dot prod of \( s(x) \) & \( g(x) \) small \( x \) would be

\[ \sum_{n=0}^{\infty} s(x) g(x) \, dx \equiv \langle s | g \rangle \]
OK.... extended dot product from
Finite $\infty$ dimensional space
(i.e. 1, 2, 3...)
to continuous $\infty$ dimensional space

\[
\sum_{n=0}^{\infty} x_n \phi_n = \langle \phi | \psi \rangle
\]

Almost!
in inner product in finite space

But wait... need a bit more to extend idea of dot prod

in V.S. $|\vec{A}|^2 = \vec{A} \cdot \vec{A}$

But really we've allowed complex #s
so need

$|\vec{A}|^2 = \vec{A}^* \cdot \vec{A}$

so we need

\[
\sum_{n=0}^{\infty} \overline{f(x)} g(x) dx = \langle \phi | \psi \rangle
\]

This IS def of inner product in V.S.

$\langle \text{dogs} | \text{cats} \rangle = \int \overline{\text{dogs}}(x) \text{cats}(x) dx$
\[ \Delta \cdot \vec{d} = A \cdot \vec{b} + d \vec{y} \]

also had

\[ \vec{e} \cdot \vec{b} = \{0, 0, 0\} \]

ie.

def of orthogonal

is there

Some thing

in F. 5. ?

\[ \Rightarrow \text{YES!} \]

\[ \sum_{n=0}^{\infty} g_n(x) \sin(nx) = \{0, 0, \ldots, 0\} \]

Then \( S(x) \) \( \perp g(x) \) are \( \perp \)
in F. 5.

Now: Not all complete basis

in F. 5. have this property!

exit polynomials of order \( n \), \( x^n \)

= complete, perfect basis

set in F. 5.

As a matter of fact, Taylor series work because

\( x^n \)'s = Span funct space \( f \in \mathbb{R}^\infty \)

\[ S(x) = S(x) x^0 + \frac{dx}{dx} x^1 + \frac{d^2x}{dx^2} x^2 + \cdots \]

But clearly \( \int x^0 x^1 x^2 x^3 \cdots \) do not

\[ \Rightarrow \int S(x)(x^n) dx = 0 \]

So \( x^n \)'s are \( \perp \) in F. 5.
However, Legendre Polynomials which are built from polynomials \( x^n \) do satisfy this condition.

The Big Point is this----

Some basis in F.S. are complete basis AND have an inner product that acts just like VECTORS.

Such Function Space Basis That Have All Properties of Vectors

1) Complete
2) Have Inner Products

= Hilbert Function Spaces.

Next --- Big deal
Keeping this in mind:

Schrödinger's equation

\[ \hat{H} \psi = E \psi \]

We demand separable (i.e., \( \psi \neq \psi(x) \))

energy eigenstate solutions which reduces then to

\[ \hat{H} \psi(x) = E \psi(x) \]

\[ \Rightarrow \psi(x) \sim e^{-i \frac{E}{\hbar} x} \psi(0) \]

Condition of Born's probability

That \( \psi \) be square integrable

(see Normalizable)

All of these conditions on \( \psi \) require \( \psi \) to be part of a complete BASIS set.

We can always make them such that they satisfy the inner product condition.

Thus, \( \psi \) is entirely built on From a Hilbert space

which are complete and \( \langle \psi | \psi \rangle = 1 \). There for harder

Solutions in the future can be constructed from these

& Great Solutions that act as complete Basis
So solving $\hat{H}\psi = E\psi$, the time independent form we get $\psi(x,t) = e^{-iE\frac{t}{\hbar}}\psi(x)$.

That is complete 1 basis set to use, when doing very advanced techniques to solve more difficult problems.

Techniques:

1) Time independent perturbation
2) Time dependent perturbation
3) Variational calculations

So huge!

It is also the connection between matrix & wave mechanics:

- Abstract complex waves & wave packets = Hilbert complex vectors
- Any properties of vectors

Schrödinger 1926 just after his wave & Heisenberg matrix papers
\[ \psi_1(x) = e^{-\frac{x^2}{2}}, \quad \psi_2(x) = xe^{-\frac{x^2}{2}} \]

Huh?

\[ \langle \psi_1(x) | \psi_2(x) \rangle = \int_{-\infty}^{\infty} \psi_1^* \psi_2 \, dx \]

\[ = \int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} \cdot xe^{-\frac{x^2}{2}} \, dx = \int_{-\infty}^{\infty} xe^{-x^2} \, dx \]

well

\[ S(x) = x \]

\[ S(x) = 1 \quad S(x) \text{ is odd} \]

\[ \therefore \]

\[ S(x) = \frac{1}{e^{x^2}} \]

\[ \therefore \]

\[ S(\text{odd})(\text{even}) \, dx = S(\text{odd}) \, dx = 0 \quad \text{symm.} \]

which is always = 0

so

\[ \langle \psi_1 | \psi_2 \rangle = 0 \]
OK: The point is our QM formalism has been based on $\Psi$'s that are Hilbert space's & thus can think of as sort of vectors

\[ \int_{-\infty}^{\infty} |\Psi|^2 \, dx = 1 = \text{Born's probabilistic condition} \]

Can be rewritten as

\[ \langle \Psi | \Psi \rangle = 1 \]

Also: Expectation value calculations

\[ \langle \mathbf{0} \rangle = \int_{-\infty}^{\infty} \Psi^* \mathbf{0} \Psi \, dx \]

why not

\[ \langle \mathbf{0} \rangle = \langle \Psi | \mathbf{0} | \Psi \rangle \geq \text{Sure!} \]

except we know (now) order is

huge for $\Psi$

Thus is +
\[ \langle 0 | \psi \rangle = \langle \psi | 0 \rangle \]

or

\[ = \langle \psi^* | \psi \rangle \]

interpret as

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

Well ... let's invent a procedure to make them both work!

Inventing shouldn't bother you

--- recall from \[ |A| = A\ast \bar{A} \]

is complex

had to

invent complex \[ |Z| = Z\ast \bar{Z} \]

conjugate

OK so here is the deal: --

For

\[ \langle 0 | \psi \rangle = \langle \psi | 0 \rangle = \langle \circ \psi | \psi \rangle \]

\[ = \int |p\rangle \psi^* \psi \, dp = \int |\circ \psi^* \psi \rangle \, dp \]

need to

\[ \ast \]

no surprise

but also transpose!
So \((\hat{\mathbf{C}})^{\dagger}\) is then completed conjugated. Together,
\[
\hat{\mathbf{C}}^\dagger = \hat{\mathbf{C}}^T
\]
adjoint

take the adjoint of
\(\hat{\mathbf{C}}\) \(\Rightarrow\)’s transpose & complex conjugate

meaning will be come clearer later when we look at all of these as matrices, not functions.
So for now, just remember.

\[
\langle \phi | \psi \rangle = \int_{-\infty}^{+\infty} \hat{\mathbf{C}}^{\dagger} \psi^* \phi \, dx
\]

\[
= \int_{-\infty}^{+\infty} \hat{\mathbf{C}}^T \psi^* \phi \, dx
\]

\[
= \int_{-\infty}^{+\infty} \hat{\mathbf{C}} \psi \phi^* \, dx
\]

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

For example...
\[ D = \frac{1}{dx}, \quad \text{and} \quad D^+ \]

Start:

\[ \langle \phi | D \psi \rangle = \int_{-\infty}^{+\infty} \phi^* \left( \frac{1}{dx} \psi \right) dx \]

Integrate by parts:

\[ \int udv = uv - \int v du \]

\[ u = \phi^*, \quad \frac{du}{dx} = \frac{d\phi^*}{dx} \]

\[ dv = \frac{1}{dx} \psi = \frac{\psi}{dx} \quad \text{so} \quad du = \frac{d\phi^*}{dx} dx \]

So:

\[ \int udv = \int v du \]

\[ v = \psi \]

\[ \langle \phi | D \psi \rangle = \phi^* \psi \left|_{-\infty}^{+\infty} \right. - \int_{-\infty}^{+\infty} \frac{d\phi^*}{dx} \psi dx \]

New both:

\[ \phi \text{ and } \psi \text{ must go} \]

\[ \text{and} \quad \psi \text{ goes} \]

Physical problem:

So:

\[ \langle \phi | D \psi \rangle = \int_{-\infty}^{+\infty} \left( -\frac{d}{dx} \right) \phi^* \psi dx \]

\[ = \langle -\frac{d}{dx} \phi^* | \psi (x) \rangle = \langle D^+ \phi | \psi \rangle \]

Or:

\[ D^+ = -\frac{d}{dx} = \text{adjoint } D \]

\[ D = D^+ \]
Now is it possible to have

\[ \langle \psi_1, \hat{D} \psi_2 \rangle = \langle \psi_2, \hat{D}^+ \psi_1 \rangle \]

such that \( \hat{D} = \hat{D}^+ \) ?

In other words

\( \hat{D} \)'s whose adjoint is the \( \hat{D} \)?

The answer is \textbf{YES} \& it will be very important for us.

So when \( \hat{D}^+ = \hat{D} \) \textbf{self-adjoint} or \textbf{Hermitian} \( \hat{D} \)?
Why are Hermitian (self-adjoint) operators significant?
by ax:

Consider position \( \vec{x} \), \( \vec{X} = X \)

First send \( \vec{x} \)

\[
\langle \psi_1 | \vec{x}^2 | \psi_2 \rangle = \int_{\mathbb{R}} \psi_1^* \psi_2 \, d\vec{x}
\]

\[
= \int_{\mathbb{R}} \psi_1^* \psi_2 \, d\vec{x}
\]

\[
= \int_{\mathbb{R}} \vec{x}^2 | \psi_1 \rangle \langle \psi_2 | \vec{x} \rangle
\]

key

\( \vec{x}^2 = X \)

\( \vec{X} \) is Hermitian!

That's a clue... position is an observable!

It turns out all observables eigenvalues & expectations of observables must be Hermitian!

Why?
Hermitean $\hat{q}$'s have

\[ \forall \text{ real values } \hat{q}, \text{ i.e. } \hat{q} = \text{ Hermitian} \]

\[ \langle \hat{q} \rangle = \langle \hat{q} \hat{q} \rangle \]
\[ \text{ i.e. } \langle \hat{q} \rangle = \text{ real} \]
\[ \text{ if most } = \langle \hat{q} \hat{q} \rangle \]

\[ \langle \hat{q} \rangle^* = \langle \hat{q}^\dagger \hat{q} \rangle \]

But is $\hat{q}^\dagger$ = Hermitian = $\hat{q}^\dagger$

\[ \langle \hat{q} \hat{q} \rangle = \langle \hat{q} \rangle^* = \langle \hat{q} \hat{q} \rangle = \langle \hat{q} \rangle \]

\[ \therefore \langle \hat{q} \rangle^* = \langle \hat{q} \rangle \text{ only if } \langle \hat{q} \rangle = \text{ real} \]

1. $\hat{q} = \text{ eigenvalues of } \hat{q}$

Then $\hat{q} \psi = \psi \hat{q}$

\[ \langle \psi | \hat{q} | \phi \rangle = \langle \phi | \hat{q} | \phi \rangle \]
\[ \langle \psi | \hat{q} | \phi \rangle = \langle \phi | \hat{q} | \phi \rangle \]
\[ \langle \psi | \hat{q}^\dagger | \phi \rangle = \langle \phi | \hat{q} | \phi \rangle \]
\[ \langle \phi | \hat{q}^\dagger | \phi \rangle \geq 0 \text{ only if } \langle \phi | \hat{q} | \phi \rangle = \text{ real} \]
Conclude: Risk in a nutshell.

\[ \hat{\mathbf{P}} = \frac{1}{2} \mathbf{1} \]

\[ \mathbf{A} \mathbf{H} = \mathbf{E} \mathbf{H} + \mathbf{B} \mathbf{H} \]

Demand eigenvectors

So: \( \mathbf{E} \mathbf{H} + \mathbf{B} \mathbf{H} \)

Prove

Because it's true

real eigenvalues

Because it's true

\( \mathbf{H} \) is Hermitian