E.F. Deveney / BSC Physics: PH402 Quantum I

Note Title

Linear Algebra in Q.M. Part 2

Scherrer C5

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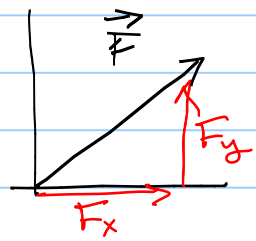
Vector & Function Spaces

* recasting our Q.M. formalism using Linear Algebra ---

introduce Hermetian or Self-adjoint Ô's & role in Q.M.

We'll start by reviewing what we already know about V.S. & F.S.'s

V.S.



$\vec{F} = F_x \hat{i} + F_y \hat{j}$

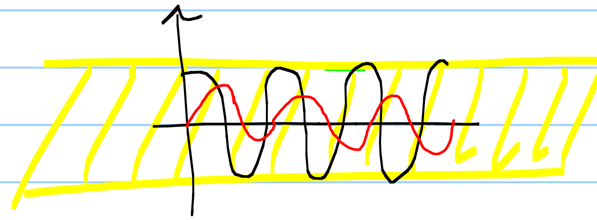
or just

$\vec{F} = (F_x, F_y)$

$\hat{i}$ & $\hat{j}$ = Linearly indep basis that completely "spans" 2-D

$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ row reduced echelon from Gaussian elimination

F.S.



$$f(x) = \sum_{n=0}^{\infty} [a_n \cos(n\omega x) + b_n \sin(n\omega x)]$$

= Fourier Series or:

$$f(x) = \int_{-\infty}^{+\infty} f(k) e^{ikx} dx$$

= Fourier Integral

Sin's & Cos's = ∞-D Linearly indep Basis that completely "Fills" all of funct space (ie WRONSKIAN $\neq 0$)

Introduce The dot product $\equiv$ Inner Product in F.S.

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

where

$\hat{e}_i \cdot \hat{e}_j = \begin{cases} 0; & j \neq i, \text{ ex. } \hat{x} \cdot \hat{y} = 0 \\ 1; & j = i, \text{ ex. } \hat{x} \cdot \hat{x} = 1 \end{cases}$

Now if had ∞ V.S. dot prod would Like

$A_1B_1 + A_2B_2 + A_3B_3 + \cdots A_\infty B_\infty$

extend to F.S. which is ∞

here not vectors $(\vec{A}, \vec{B})$ But functions, say $f(x)$, $g(x)$

so the ∞ dot prod of $f(x)$ & $g(x)$ for all x would be

$f(1)g(1) + f(2)g(2) + \cdots f(\infty)g(\infty)$

or

$$\int_{-\infty}^{+\infty} f(x) g(x) dx \equiv \langle f | g \rangle$$

OK .... extended dot
product from
Finite ∞ dimensional space
(ie 1, 2, 3 ...)
to continuous ∞ dimensional space

$$\underbrace{\int_{-\infty}^{+\infty} f(x)\,g(x)\,dx \;\}\equiv \langle f|g\rangle}_{\text{Almost!}}$$

inner product in funct 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 recall, we've allowed complex #'s
so need
$$|\vec{A}|^2 = \vec{A}^*\cdot\vec{A}$$

so we need

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

this $\underline{\underline{\text{IS}}}$ def of inner
product in F.S.

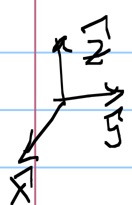
$$\langle \text{dogs}|\text{cats}\rangle = \int (\text{dogs})^*(\text{cats})\,dx$$

Now

V.S.

$\vec{A}\cdot\vec{B} = A_xB_x + A_yB_y$

also had



$$\hat{e}_i\cdot\hat{e}_j = \begin{cases} 0, & i\neq j \\ 1, & i=j \end{cases}$$

i.e.
def of orthogonal
is there
same thing
in F.S.?

F.S

$g(x)$, $f(x)$

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

Yes!

$$\int_{-\infty}^{+\infty} f^*(x)\, g(x)\, dx = \begin{cases} 0, & f(x)\neq g(x) \\ 1, & f(x)=g(x) \end{cases}$$

Then $f(x)$ & $g(x)$ are $\perp$ in F.S.

Now: Not all complete basis in F.S. have this property!

ex: polynomials of order n, x^n = complete, perfect basis set in F.S.

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as a matter of fact Taylor Series work because x^n's = span funct space & so

$$f(x) = f(x_0)x^0 + \frac{df}{dx}x^1 + \frac{1}{2}\frac{d^2f}{dx^2}x^2 + \ldots$$

But clearly $x^0, x^1, x^2, x^3 + \ldots$ do not satisfy $\int_{-\infty}^{+\infty}(x)(x^2)\,dx = 0$ $\Big\}$ so x^n's are not $\perp$ in F.S.

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...

Schrö Q.M. $\Rightarrow$ $\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$

we demand separable (ie $V \neq f(t)$)

energy eigenstate solns which reduces then to

$\hat{H}\psi(x) = E_n \psi(x)$

s.o. $\Psi = e^{-i\frac{E}{\hbar}t}\psi(x)$

+

Condition of Born's prob interp

That ψ's be Square integrable (ie Normalizable)

All of these conditions on Ψ require Ψ's That are part of a complete BASIS set & we can always make them such that they satisfy the inner product condition

Thus $\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$ is entirely built on Ψ from a Hilbert Space

When we do
time dep perturbation
time indep perturbation & variational calcs

which are Complete and $\perp$. Therefor Harder Solns in The Future Can be constructed from these Great Solns That act as complete Basis

So solving $\hat{H}\psi = E\psi$, the time indep easiest form

we get $\Psi(x,t) = e^{-i\frac{E_n}{\hbar}t}\psi(x)$

That are complete $\perp$ basis set to use when doing

Very advanced techniques to solve more difficult problems

Techniques:

1.) time indep perturbation

2.) time dep perturbation

3.) variational calculations

So HUGE!

Schrö 1926 just after his wave & Heisenberg's matrix papers

It is also the connection between

Matrix & Wave Mechanics

abstract complex vector = complex wavefuncts = $\underbrace{\text{Hilbert}}$

thus have all properties of vectors

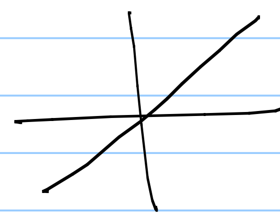
ex: $\psi_1(x) = e^{-x^2/2}$, $\psi_2(x) = x e^{-x^2/2}$

what is

$$\langle \psi_1(x) | \psi_2(x) \rangle = ? = \int_{-\infty}^{+\infty} \psi_1^* \psi_2 \, dx$$

$$= \int_{-\infty}^{+\infty} \left(e^{-x^2/2}\right)^* x e^{-x^2/2} \, dx = \underbrace{\int_{-\infty}^{+\infty} x e^{-x^2} dx}_{\text{Huh?}}$$

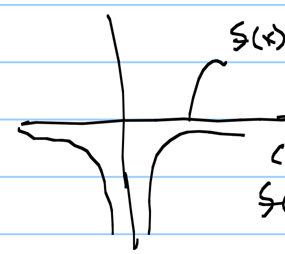
well



$f(x) = x$

, clearly $f(x) = -1\, f(-x)$ ie odd

&

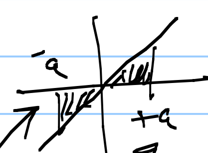


$f(x) = \frac{1}{e^{x^2}}$

clearly $f(x) = +1\, f(-x)$ ie even

so

$$\underbrace{\int}_{\text{symmetric BC}} (\text{odd})(\text{even})\, dx = \underbrace{\int}_{\text{sym}} (\text{odd})\, dx =$$



$-a$ $+a$

which is always $= 0$

so

$$\boxed{\langle \psi_1 | \psi_2 \rangle = 0}$$

OK: Big point is our Q.M. formalism has been based on Ψ's that are Hilbert space's & thus can think of as sort of vectors

& therefore use lots of linear algebra.

For examples:

$$\int_{-\infty}^{+\infty} \psi^* \psi \, dx = 1 \quad = \text{Born's probabilistic condition}$$

can be rewritten as

$$\langle \psi | \psi \rangle = 1$$

Also: Expectation value calculations

$$\langle o \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{o} \psi \, dx$$

why not

$$\langle o \rangle = \langle \psi | \hat{o} | \psi \rangle \Big\} \text{ SURE!}$$

except we now know order is huge for $\hat{o}$'s

This is it

$\langle O \rangle = \langle \psi | \hat{O}\psi \rangle$

or

$= \langle \psi \hat{O} | \psi \rangle$

interpret as

$= \langle \hat{O}\psi | \psi \rangle$

well ---- Lets invent procedure to make them Both work!

Inventing shouldn't bother you --- recall seen $|A|^2 = \vec{A}\cdot\vec{A}$

is complex had to invent complex conjugate $|z|^2 = z^* z$

OK so here is the deal ---

For

$\langle O \rangle = \langle \psi | \hat{O}\psi \rangle = \langle \hat{O}\psi | \psi \rangle$

$= \int_{-\infty}^{+\infty} \psi^* \hat{O} \psi \, dx = \int \underbrace{\hat{O}}_{\text{need to}} \psi^* \psi \, dx$

$\hat{O}^*$ no surprise

but also transpose!

So $\left(\hat{O}^{\text{Transposed}}\right)^*$

Then complexed conjugated

together

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

adjoint

take the adjoint of $\hat{O}$ ⇒ 's Transpose & complex conjugate

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

OK Then

$$\langle o \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{O} \psi \, dx = \int_{-\infty}^{+\infty} (\hat{O}^{T*}) \psi^* \psi \, dx$$

$$= \int_{-\infty}^{+\infty} \hat{O}^{\dagger} \psi^* \psi \, dx$$

$$= \langle \psi | \hat{O} | \psi \rangle \equiv \langle \hat{O} \psi | \psi \rangle$$

For example ...

Example of Adjoint $\hat{O}$

$\hat{D} = \frac{d}{dx}$, find $\hat{D}^+$

start $\langle \phi | D\psi \rangle = \underbrace{\int_{-\infty}^{+\infty} \phi^* \left(\frac{d}{dx}\psi\right) dx}_{\text{integrate by parts}}$

$\int u\,dv = uv - \int v\,du$

$u = \phi^*$; $\frac{du}{dx} = \frac{d\phi^*}{dx}$ so $du = \frac{d\phi^*}{dx}d$

$dv = \frac{d\psi}{\cancel{dx}}\cancel{dx} = d\psi$

so

$\int dv = \int d\psi$

$v = \psi(x)$

$\langle \phi | D\psi \rangle = \underbrace{\phi^*(x)\psi(x)\Big|_{-\infty}^{+\infty}}_{\substack{\text{now both} \\ \phi \,\&\, \psi \text{ must} \to 0 \\ @ \pm\infty \text{ for} \\ \text{physical} \\ \text{problem}}} - \int_{-\infty}^{+\infty} \frac{d\phi^*}{dx}\psi(x)\,dx$

so

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

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

or $D^+ = -\frac{d}{dx}$ = Adjoint $\hat{O}$ of $D = D^+$

Now: is it possible to have

$$\langle \psi_1 | \hat{O} \psi_2 \rangle = \langle \hat{O}^\dagger \psi_1 | \psi_2 \rangle$$

such that $\hat{O} = \hat{O}^\dagger$?

in other words

$\hat{O}$'s whose adjoint = the $\hat{O}$

?

The answer is YES & it will be very important for us.

So when $\hat{O}^\dagger = \hat{O}$ = self adjoint

or

HERMETIAN $\hat{O}$

why?

why are Hermetian (self adjoint) $\hat{o}$'s significant?
by ex:

consider position $\hat{o}$, $\hat{x} = x$

1^{st} find $\hat{x}^{+}$

$$\langle \psi_1 | \hat{x} | \psi_2 \rangle = \int_{-\infty}^{+\infty} \psi_1^{*} x \psi_2 \, dx$$

$$= \int_{-\infty}^{+\infty} x \, \psi_1^{*} \psi_2 \, dx$$

$$= \langle \hat{x}^{+} \psi_1^{*} | \psi_2 \rangle$$

hey $\hat{x}^{+} = x$

$\hat{x}$ is Hermetian!

Thats a clue..... position = an observable!

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

why?

Hermetian $\hat{O}$'s have

REAL → expectation values & eigenvalues! → All Real world!

* proof consider $\hat{q}^{\dagger} = \hat{q}$, ie $\hat{q}$ = Hermetian

1) Expectation of Hermet = REAL

$\langle q \rangle = \langle \psi | \hat{q} | \psi \rangle$ is $\langle q \rangle$ = real

it must $= \langle q \rangle^*$

can show

$\langle q \rangle^* = \langle \psi | \hat{q}^{\dagger} | \psi \rangle$

But if $\hat{q}^{\dagger}$ = Hermetian $= \hat{q}$

$\langle q \rangle^* = \langle \psi | q | \psi \rangle = \langle q \rangle$

$\therefore$ $\langle q \rangle^* = \langle q \rangle$ only if $\langle q \rangle$ = real

2) eigenvalues of Hermetian = REAL

if ψ = eigen funct of $\hat{q}$

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

$\langle \psi | \hat{q}\,\psi \rangle = \langle q\,\psi | \psi \rangle$

$\langle \psi | q\,\psi \rangle = \langle q^*\,\psi | \psi \rangle$

$q \langle \psi | \psi \rangle = q^* \langle \psi | \psi \rangle$

$q = q^*$ only if q = real

Conclude: Q.M. in a Nutshell!

$$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

demand energy eigenstates $\rightarrow$ so $\hat{H}\psi = E_i\psi$ + Born

so $\Psi = e^{-i\frac{E_I}{\hbar}t}\psi(x)$

$\underbrace{= \text{Stationary}}$

= Bases to Build more complicated problems

$\hat{H} = \frac{P^2}{2m} + V + \{H'\}$

or time dependent problems

means ψ = Hilbert

so $\langle\psi|\psi\rangle = 1$

preserve probability

implies ψ_s = Hilbert

$\langle o\rangle = \langle\psi|\hat{o}|\psi\rangle$

& $\hat{o}$ are Hermetian

$\hat{o}^+ = \hat{o}$

because they give real eigen values & real expectations