Phys 521 Fall 2023
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Lecture #1 Some Math

Quantum position states are vectors in an abstract space of complex functions with a (Unitary) inner product: Hilbert space.

Euclidean vectors: $\vec{r} \doteq (x_1, x_2, x_3)$ coordinate

$\vec{r} \cdot \vec{r} = (x_1^2 + x_2^2 + x_3^2)$ norm

norm invariant under rotation.

orthogonal, unit vectors

$$\hat{e}_i \cdot \hat{e}_j = \delta_{ij}$$

$$\vec{r} = \sum_{i=1}^{3} x_i \hat{e}_i$$

Dirac vector notation: $|v\rangle$ "ket"

Linear vectorspace $\{|v\rangle\}$

① addition $|c\rangle = |a\rangle + |b\rangle$

② scalar multiplication distributive over vectors

$$a(|v\rangle + |w\rangle) = a|v\rangle + a|w\rangle$$

③ scalar multiplication distributive in scalars

$$(a+b)|v\rangle = a|v\rangle + b|v\rangle$$

④ scalar multiplication associative

$$a(b|v\rangle) = ab|v\rangle$$

⑤ addition commutative

$$|v\rangle + |w\rangle = |w\rangle + |v\rangle$$

⑥ addition associative

$$|v\rangle + (|w\rangle + |z\rangle) = (|v\rangle + |w\rangle) + |z\rangle$$

(7) exists null vector $|0\rangle + |v\rangle = |v\rangle$

(8) exists inverse under addition

$$|v\rangle + |-v\rangle = |0\rangle$$

Linear independence

Set of N vectors $|i\rangle$ such that any vector may be expanded

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

N = dimension of space

$\{|i\rangle\}$ form a basis.

c_i = complex numbers

Components c_i represent vector as column

$$|v\rangle \doteq \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}_{i\text{-basis}}$$

Inner Product and Dual Space

Euclidean vector

$$\vec{A} \cdot \vec{B} = \underbrace{(A_1, A_2, A_3)}_{\text{"}\vec{A}\cdot\text{"}} \begin{pmatrix} B_1 \\ B_2 \\ B_3 \end{pmatrix}$$

"A·" linear map of vectors to scalars.

Generalize linear map

$$|v\rangle \xrightarrow{\langle w|} \text{scalar}$$

these maps form a linear vector space called the dual space with elements $\langle w|$ "bra"
Every vector has a dual

$$|v\rangle \doteq \begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix} \qquad \langle v| \doteq (v_1^*, v_2^*, \ldots v_N^*)$$

The <u>Dirac bracket</u> is the inner product

$$\langle v|w\rangle = (v_1^*, v_2^*, \ldots v_N^*) \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix}$$

Product is

1. $\langle v|w\rangle = \langle w|v\rangle^*$ skew symmetric
2. $\langle v|v\rangle \geq 0$ equality iff $|v\rangle = |0\rangle$
3. $\langle v|\big(\underbrace{a|w\rangle + b|z\rangle}_{=|aw+bz\rangle}\big) = a\langle v|w\rangle + b\langle v|z\rangle$

$$\langle aw+bz|v\rangle = \langle v|aw+bz\rangle^*$$

$$= a^*\langle w|v\rangle + b^*\langle v|z\rangle \quad \text{anti-linear}$$

convenient to choose ortho-normal basis $\{|i\rangle\}$

$$\langle i | j \rangle = \delta_{ij}$$

Gram-Schmidt construction

complete basis $\{|b_i\rangle\}$

$$|1\rangle = \frac{|b_1\rangle}{\sqrt{\langle b_1 | b_1 \rangle}}$$

$$|2'\rangle = |b_2\rangle - |1\rangle \langle 1 | b_2 \rangle$$

normalize $\quad |2\rangle = \dfrac{|2'\rangle}{\sqrt{\langle 2' | 2' \rangle}}$, etc.

Schwartz Inequality

$$|\langle v | w \rangle| \le \sqrt{\langle v | v \rangle} \sqrt{\langle w | w \rangle}$$

complex norm $|c| \equiv \sqrt{c^* c}$

triangle norm $\left| |v\rangle \right| \equiv \sqrt{\langle v | v \rangle}$

$$\left| |v\rangle + |w\rangle \right| \le \left| |v\rangle \right| + \left| |w\rangle \right|$$

Subspace subset of vector space forming its own vector space.

Linear Operators

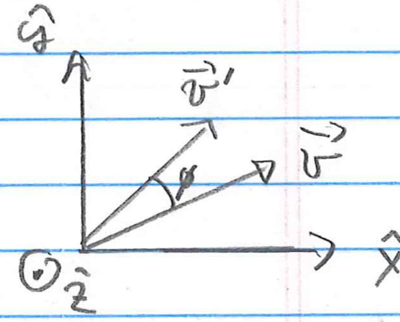
linear map $|v\rangle \xrightarrow{\hat{T}} |v'\rangle$

I often use "hat" to denote operators.

$$\hat{T}\left(a|a\rangle + b|b\rangle\right) = a\left(\hat{T}|a\rangle\right) + b\left(\hat{T}|b\rangle\right)$$

Example! Rotation of Euclidean vector

$$\hat{R}(\phi\hat{z}) \doteq \begin{pmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



$c \equiv \cos\phi$

$s \equiv \sin\phi$

active as opposed to passive change of basis

$$\hat{R}^E(\theta\hat{y})\,\hat{R}_z(\phi\hat{z}) \neq \hat{R}_z^E\,\hat{R}_y$$ rotations do not commute

define commutator:

$$[\hat{S}, \hat{T}] \equiv \hat{S}\hat{T} - \hat{T}\hat{S}$$

Projection operators. In basis $\{|i\rangle\}$

$$|v\rangle = \sum v_i |i\rangle \doteq \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}$$

$$\langle i|v\rangle = \sum_j v_j \underbrace{\langle i|j\rangle}_{\delta_{ij}} = v_i$$

So $|v\rangle = \sum |i\rangle\langle i|v\rangle$

$$\hat{I} = \sum |i\rangle\langle i| \quad \text{unit operator}$$

$$\hat{P}_i = |i\rangle\langle i| \quad \text{projection operator}$$

In basis, operators represented as matricies

$$|v'\rangle = \hat{T}|v\rangle = \sum_j \hat{T}|j\rangle\langle j|v\rangle$$

$$\langle i|v'\rangle = \langle i|\hat{T}|v\rangle$$

$$= \sum_j \underbrace{\langle i|\hat{T}|j\rangle}_{[T]_{ij}}\langle j|v\rangle$$

$$v'_i = \sum_j [T]_{ij}\, v_j \quad \text{sum on column index}$$

$$\begin{pmatrix} v_1' \\ v_2' \\ \vdots \\ v_N' \end{pmatrix} = \Big[\ T_{ij}\ \Big] \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}$$

Corresponding bra transforms as

$$|v'\rangle = \hat{T}\,|v\rangle$$

$$\langle v'| = \langle v|\,\hat{T}^{+}$$

Define Hermitian conjugate

$$\hat{T}^{+} \doteq \left(T_{ij}^{*}\right)^{T}$$ transpose

or $$T_{ij}^{+} = T_{ji}^{*}$$

Example: Pauli matrix

$$\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \hat{\sigma}_y^{+}$$

$$\hat{T}^{+} = \hat{T}$$ Hermitian matrix

just as any complex number

$$c = \underbrace{\frac{c+c^*}{2}}_{\text{real}} + \underbrace{\frac{c-c^*}{2}}_{\text{imaginary}}$$

any

$$\hat{T} = \underbrace{\frac{\hat{T}+\hat{T}^{+}}{2}}_{\text{Hermitian}} + \underbrace{\frac{\hat{T}-\hat{T}^{+}}{2}}_{\text{anti-Hermitian}}$$

$$A^{+} = A \qquad\qquad A^{+} = -A$$

Important! easy to show that

Eigenvalues of Hermitian matrix are real

Observables correspond to Hermitian operators

Unitary operator $\hat{U}^+ \hat{U} = \hat{I}$

Dirac product invariant under unitary transformation

$$\hat{U} |v\rangle = |v'\rangle$$

$$\hat{U} |w\rangle = |w'\rangle$$

$$\langle w' | v' \rangle = \langle w | U^+ U | v \rangle = \langle w | v \rangle$$

Functions of operators.

Defined by Taylor expansion

$$f(\hat{A}) = \sum_{i=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=0} \hat{A}^n$$

Any unitary operator can be written as

$$\hat{U} = e^{i\hat{H}} \qquad \hat{H} \text{ Hermitian}$$

Example: rotation operator are unitary

$$R^{\dagger}(\theta\hat{n}) = R^{-1}(\theta\hat{n}) = R(-\theta\hat{n})$$

$$R(\theta\hat{n}) = e^{-i\theta\hat{n}\cdot\vec{T}}$$

$\hat{T}_i$ $i=1,2,3$ are Hermitian generators

Example of Lie group pronounced "lee" continuous transformations. Almost all (and in particular relevant to us) properties follow from

$$[\hat{T}_i, \hat{T}_j] = i\sum_k \underbrace{f_{ijk}}_{\text{structure constants}} \hat{T}_k$$

For quantum rotation group SU(2)

Det = 1, unitary $2^2-1=3$ generators

$$\left[\frac{\sigma_i}{2}, \frac{\sigma_j}{2}\right] = i\sum_k \varepsilon_{ijk}\frac{\sigma_k}{2}$$

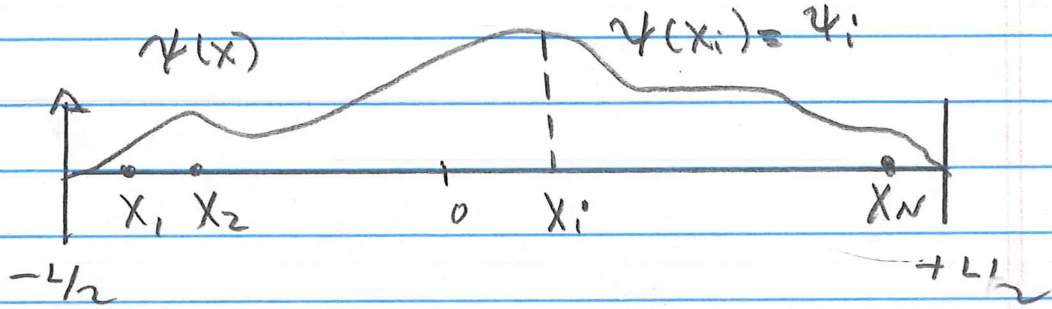
Einstein summation:
repeated indices assumed to be summed.
no need to write Sum symbol

lowest rep. is 2x2 matrices

σ_i pauli matrices $\frac{\sigma_i}{2}$ generators

structure constants just completely antisymmetric ε_{ijk} symbol

Hilbert Space An ∞ dimension, non denumerable vector space with complex functions as vectors.



N equally spaced points, N+1 equal spaces of size

$$\Delta \equiv x_{n+1} - x_n = \frac{L}{N+1}$$

$$x_n = -\frac{L}{2} + n\left(\frac{L}{N+1}\right)$$

$$x_0 = -\frac{L}{2}, \; x_1 = -\frac{L}{2} + \Delta, \ldots, x_N = \frac{L}{2} - \Delta, \; x_{N+1} = \frac{L}{2}$$

ψ_i approximates $\psi(x)$

$$|\psi\rangle \doteq \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix}$$ form N dimensional vector space

$$|\psi\rangle + |\phi\rangle \doteq \begin{pmatrix} \psi_1 + \phi_1 \\ \psi_2 + \phi_2 \\ \vdots \\ \psi_N + \phi_N \end{pmatrix}$$

$$\langle \phi | \psi \rangle = \sum_{i=1}^{N} \phi_i^* \psi_i$$

basis vectors

$$|x_i\rangle \doteq \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$ i^{th} element 1, all others 0

$$\langle x_i | x_j \rangle = \delta_{ij}$$

$$\psi(x_i) = \psi_i = \langle x_i | \psi \rangle$$

$$|\psi\rangle = \sum |x_i\rangle \psi(x_i) = \sum |x_i\rangle\langle x_i|\psi\rangle$$

In limit $N \to \infty$ our inner product diverges. We should multiply by normalization factor $\Delta = \frac{L}{N+1}$

$$\langle \phi | \psi \rangle = \lim_{N\to\infty} \sum_{i=1}^{N} \Delta \, \phi^*(x_i) \psi(x_i)$$

$$= \int_{-L/2}^{L/2} dx \, \phi^*(x) \psi(x)$$

Can also take $L \to \infty$ if needed

$$\hat{I} = \int dx \, |x\rangle\langle x|$$

$$\langle x_i | x_j \rangle = \delta_{ij} \xrightarrow{\text{limit}} \langle x' | x \rangle = \delta(x' - x)$$

Dirac δ- function not really a function, but represented by any function with property

$$\int_{-a}^{+a} f(x)\,\delta(x)\,dx = f(0)$$

"Spike" at $x=0$ of unit area

most useful representation:

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\,dk = \lim_{\lambda\to\infty} \frac{1}{\pi}\,\frac{\sin\lambda x}{x}$$

easy to see $\delta(0) = \lim\limits_{\lambda\to\infty} \frac{\lambda}{\pi}$

numerically, can show $\int_{-a}^{a}\delta(x)\,dx = \lim\limits_{\lambda\to\infty}\frac{1}{\pi}\int_{-a}^{a}\frac{\sin\lambda x}{x}\,dx$
$= 1$

properties ① $\delta(x) = \delta(-x)$ even

② Derivative of step $\dfrac{d\,\Theta(x-a)}{dx} = \delta(x-a)$

step $\Theta(x-a) \equiv \begin{cases} 0 & x<a \\ 1 & x>a \end{cases}$

③ $\delta\big(f(x)\big) = \dfrac{\delta(x-x_0)}{\left|\frac{df}{dx}\right|_{x=x_0}}$ where $f(x_0)=0$

④ derivative

$$\delta'(x-x') = \frac{\partial}{\partial x}(x-x') = -\frac{\partial}{\partial x'}(x-x')$$

$$\int f(x')\,\delta'(x-x')\,dx' = \frac{d}{dx}\int f(x')\,\delta(x-x')\,dx'$$
$$= \frac{df}{dx}$$

$$\int f(x')\left(-\frac{d}{dx'}\delta(x-x')\right)dx' = \int \frac{df(x')}{dx'}\,\delta(x-x')\,dx' = \frac{df}{dx}$$

integrate by parts

so $\frac{d}{dx}\delta(x-x') = \delta(x-x')\,\frac{d}{dx'}$

Derivative operator.

$D\,|f\rangle = \left|\frac{df}{dx}\right\rangle$ is not Hermitian

we can show $K = \frac{1}{i}D$ is Hermitian

$\langle g|K|f\rangle =$
$\langle g|Kf\rangle = \langle Kf|g\rangle^* = \langle f|K^\dagger|g\rangle^*$

$$\iint dx\,dx'\,\langle g|x\rangle\langle x|K|x'\rangle\langle x'|f\rangle$$
$$= \iint dx\,dx'\; g^*(x)\,\delta(x-x')\left(\frac{1}{i}\frac{d}{dx'}\right)f(x')$$
$$= \int dx\; g^*(x)\,\frac{1}{i}\frac{df}{dx}$$

$\langle f | K^\dagger | g \rangle^*$

$$= \left(\int dx \, f^* \left(\frac{1}{i} \frac{d}{dx} \right) g \right)^*$$

$$\frac{d}{dx}(f g^*) = \frac{df}{dx} g^* + f \frac{dg^*}{dx}$$

$$= -\int f \frac{1}{i} \frac{d}{dx} g^*$$ integrate by parts

$$f g^* \Big| + \int g^* \frac{1}{i} \frac{df}{dx} \, dx$$ Hermitian if end point term vanish

So in QM. wave function required to vanish at $\pm \infty$, so Hermitian momentum operator is

$$\hat{p}_x = \frac{\hbar}{i} \frac{d}{dx}$$