Phys 521
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Lecture #1: Some Math Preliminaries

Quantum position states are vectors in an abstract space of complex functions with inner product — Hilbert space.

Recall Euclidean vectors:

$$\vec{r} \doteq (x_1, x_2, x_3) \quad \text{in Cartesian coordinates}$$

$\doteq$ "represented by"

Norm invariant under rotations. Introduce orthonormal basis vectors,

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

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

Introduce Dirac abstract vector notation:

"ket" vector $|v\rangle$ element of linear vector space $\{|v\rangle\}$

1) addition $|c\rangle = |a\rangle + |b\rangle$ defined
2) complex scalar multiplication is distributive over vectors
$$a(|v\rangle + |w\rangle) = a|v\rangle + a|w\rangle$$
3) scalar multiplication is distributive over scalars
$$(a+b)|v\rangle = a|v\rangle + b|v\rangle$$

4) scalar multiplication is associative
$$a(b|v\rangle) = ab|v\rangle$$

5) vector addition is commutative

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

6) vector addition associative

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

7) existence of null vector $|0\rangle$.

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

8) existence of additive inverse $|-v\rangle$.

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

<u>Linear Independence</u> Exist set of N vectors $|i\rangle$ such that any vector may be expanded

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

c_i complex scalars
N = dimension of space

then $\{|i\rangle\}$ are said to form a <u>basis</u>.
Components c_i represent vector as a column

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

Inner Product and Dual Space

recall Euclidean vector inner product in Cartesian coordinates,

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

"$\vec{A}\cdot$" is a linear map of vectors to scalars

Generalize as

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

These maps form a linear vector space called the <u>dual space</u> with element $\langle w|$ "bra".

Every vector has a dual

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

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

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

Inner product is:

1) skew symmetric $\langle v|w\rangle = \langle w|v\rangle^*$

2) $\langle v|v\rangle = 0$ <u>iff</u> $|v\rangle = |0\rangle$

3) antilinear

$$\langle v|\big(a|w\rangle + b|z\rangle\big) = a\langle v|w\rangle + b\langle v|z\rangle$$

$$\equiv |aw+bz\rangle$$

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

$$= a^*\langle w|v\rangle + b^*\langle v|z\rangle$$

Orthonormal Basis $\{|i\rangle\}$

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

May be constructed by Gram-Schmidt procedure
Given any basis $\{|b_i\rangle\}$

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

subtract component $\parallel$ to $|1\rangle$

$$|2'\rangle = |b_2\rangle - |1\rangle\big(\langle 1|b_2\rangle\big)$$

normalize $|2\rangle = \dfrac{|2'\rangle}{\sqrt{\langle 2|2\rangle}}$

etc.

Schwartz Inequality:

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

↑ denotes complex norm $|C| \equiv \sqrt{C^*C}$

and $||v\rangle| \equiv \sqrt{\langle v|v\rangle}$

Triangle Inequality

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

Subspace Subset of vector space forming its own vector space.

Linear Operators

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

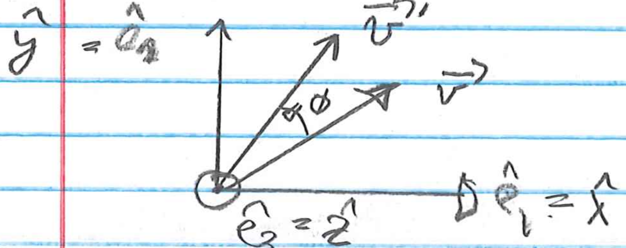
often use "hat" to denote operators for clarity.

linearity: $\hat{T}(a|v\rangle + b|w\rangle)$

$$= a(\hat{T}|v\rangle) + b(\hat{T}|w\rangle)$$

Example of linear operator - rotation of Euclidean vector.

active rotation - rotates vector
passive rotation - rotates basis



note: "hat" also denotes unit vector

active right-handed rotation by angle ϕ

operator represented by matrix

$$\hat{R}^E(\phi\hat{z}) \doteq \begin{pmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{array}{l} c \equiv \cos\phi \\ s \equiv \sin\phi \end{array}$$

$$v_1' = c v_1 - s v_2 \quad , \text{ etc.}$$

Rotations do not commute

$$\hat{R}^E(\theta\hat{y})\,\hat{R}^E(\phi\hat{z}) \neq \hat{R}^E(\phi\hat{z})\,\hat{R}^E(\theta\hat{y})$$

Define commutator bracket:

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

<u>identities:</u> $[a, b+c] = [a,b] + [a,c]$
(drop hats) $[a, bc] = b[a,c] + [a,b]c$
$[ab, c] = a[b,c] + [a,c]b$

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

$$|v\rangle = \sum_j v_j |j\rangle \doteq \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}$$

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

so completeness is

$$|v\rangle = \sum_i |i\rangle\langle i|v\rangle$$

i is "dummy" index

Then unit operator can be written as

$$\hat{I} = \sum_i |i\rangle\langle i|$$

note convenient notation "$|i\rangle\langle i|$" maps vector to vector so operator in basis.

projection operator

$$\hat{P}_i = |i\rangle\langle i|$$

In basis, operators are represented as matricies

$$|v'\rangle = \hat{T}|v\rangle = \sum_j \hat{T}|j\rangle\underbrace{\langle j|v\rangle}_{v_j \text{ component}}$$

$$\langle i|v'\rangle = \sum_j \underbrace{\langle i|\hat{T}|j\rangle}_{\text{matrix } [T]_{ij}}\langle j|v\rangle$$

$$v_i' = \sum_j [T]_{ij}\, v_j$$

sums column index

or
$$\begin{pmatrix} v_1' \\ v_2' \\ \vdots \\ v_N' \end{pmatrix} = [T]_{ij} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}$$

<u>Hermitian Conjugate</u> defined by

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

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

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

matrix $T^{+}_{ij} = T^{*}_{ji}$

<u>Example</u> Pauli y-matrix

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y^{+}$$

$\hat{T}^{+} = \hat{T}$ is said to be Hermitian

Just as any complex number

$$c = \frac{c+c^*}{2} + \frac{c-c^*}{2}$$

real + imaginary

any operator

$$T = \frac{T+T^{+}}{2} + \frac{T-T^{+}}{2}$$

Hermitian anti-Hermitian

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

Eigenvalue Problem   Eigenvectors of operator Ω

$$\Omega|\omega\rangle = \omega|\omega\rangle$$

$|\omega\rangle$ eigenvector
ω eigenvalue (complex scalar)

convenient to label eigenvector with eigenvalue

then eigenvalue problem is to find ω & $|\omega\rangle$.

$$(\Omega - \omega I)|\omega\rangle = |0\rangle \quad I \equiv \text{identity operator}$$

operator $(\Omega - \omega I)$ cannot have inverse for $|\omega\rangle$ to exist. Introduce basis $\{|i\rangle\}$

$$\sum_j \langle i|(\Omega - \omega I)|j\rangle\langle j|\omega\rangle = 0$$

$$\sum_j (\Omega_{ij} - \omega\delta_{ij})\omega_j = 0 \quad \text{using matrix notation}$$

then

$\det(\Omega_{ij} - \omega\delta_{ij}) = 0$ gives characteristic equation, a polynomial in ω for N eigenvalues.

Similarity transformation; matrix S with eigenvectors as columns diagonalizes Ω as

$$S^{+}\Omega S = \mathrm{diag}(\omega_1, \omega_2 \ldots \omega_N)$$

Shankar: Hermitian and Unitary operators have N eigenvalues.
Only for Hermitian operators are eigenvalues guaranteed to be real, with orthogonql eigenvectors.

Easy to prove that eigenvalues of any Hermitian operator are real scalars. $|\omega\rangle$ normalized eigenvector.

$$\Omega|\omega\rangle = \omega|\omega\rangle \qquad (1)$$

$$\langle\omega|\Omega^{+} = \langle\omega|\Omega = \langle\omega|\omega^{*} \qquad (2)$$

operate on (1) with bra $\langle\omega|$ and on (2) with ket $|\omega\rangle$,

$$\left.\begin{array}{l}\langle\omega|\Omega|\omega\rangle = \omega \\ \langle\omega|\Omega|\omega\rangle = \omega^{*}\end{array}\right\} \quad \begin{array}{l}\omega-\omega^{*}=0 \\ \omega=\omega^{*}\end{array}$$

Eigenvectors of Hermitian operators are orthogonal

Consider two eigenvalues ω_a, ω_b of Ω,

$$\langle\omega_b|\Omega|\omega_a\rangle = \omega_a\langle\omega_b|\omega_a\rangle \qquad (3)$$
$$\langle\omega_a|\Omega|\omega_b\rangle = \omega_b\langle\omega_a|\omega_b\rangle \qquad (4)$$

take c.c. of both sides of (4):

$$\langle\omega_a|\Omega|\omega_b\rangle^{*} = \langle\omega_b|\Omega^{+}|\omega_a\rangle = \langle\omega_b|\Omega|\omega_a\rangle$$

$$= \omega_b^{*}\langle\omega_b|\omega_a\rangle \qquad (5)$$

C.C. of left hand side

then (3)−(5) gives $0 = (\omega_a-\omega_b)\langle\omega_b|\omega_a\rangle$

then $\langle\omega_b|\omega_a\rangle = 0$ if $\omega_a \neq \omega_b$. For normalized eigenvectors

$$\langle\omega_b|\omega_a\rangle = \delta_{ba}$$

<u>Unitary operator</u> $U^\dagger U = I$

The Dirac product is <u>invariant</u> under a <u>unitary transformation</u>.

$$U|v\rangle \equiv |v'\rangle$$
$$U|w\rangle \equiv |w'\rangle$$

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

<u>Functions of Operators</u> are <u>defined</u> by Taylor expansion,

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

Any <u>unitary operator</u> may be written as

$U = e^{iH}$ where <u>H is Hermitian</u>

<u>Example</u>: Euclidean rotations

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

so $R^\dagger R = I$

introduce vector $\vec{\theta} = \sum \theta_i \hat{e}_i$ Euclidean vector

Then $R(\vec{\theta}) = e^{-i\vec{\theta}\cdot\vec{T}}$ minus gives right handed rotation

Where T_i are 3 Hermitian operators called <u>generators</u>.

What is a group?

A set of elements $\{g_i\}$ with a combination rule (called group multiplication

① $g_a \circ g_b = g_c$ every pair a, b with c in group

② associative $g_a \circ (g_b \cdot g_c) = (g_a \circ g_b) \cdot g_c$

③ existence of identity element I

$I \cdot g_a = g_a \cdot I = g_a$

④ existence of inverse for every element

$g_a \cdot g_a^{-1} = g_a^{-1} \cdot g_a = I$

In general, N generators with commutators

$$[T_i, T_j] = i \sum f_{ijk} T_k$$

$\uparrow$ Hermitian; f_{ijk} real "structure constants"

The rotations in Q.M. group is SU(2).

generators of $SU(N) = N^2-1$, So 3.

A representation is an explicit set of matricies that also have generators T_i as matricies.
So $R^E(\vec{\theta})$ are explicit group elements that act on a 3-dim vector space.

$$T_i = i \frac{dR}{d\theta_i}\bigg|_{\vec{\theta}=0} = i \frac{d}{d\theta_i}(1 - i\vec{\theta}\cdot\vec{T} + \dots)_{\vec{\theta}=0}$$

Rotation Group is SU(2): det = 1, lowest dimensional (defining) representation 2×2. Group elements have det = 1.
2×2 Hermitian generators are Pauli matricies $\frac{\sigma_i}{2}$.

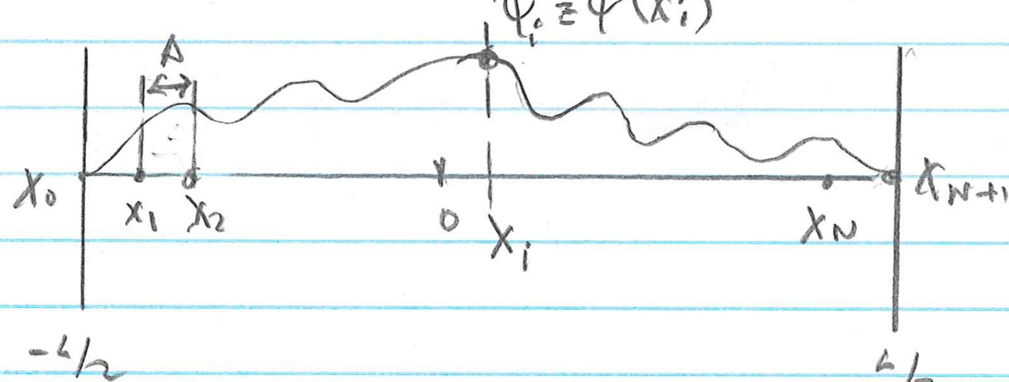
Pauli: $\sigma_x = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
traceless, Hermitian. SU(2) structure constants are ε_{ijk} completely anti-symmetric symbol: $\varepsilon_{123} = \varepsilon_{132}$ etc. $\varepsilon_{112} = 0$, etc.

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

2x2 Representation acts on a 2-dim, complex spinor:

$$\chi = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}$$

Hilbert space A non-denumerably infinite vector space with complex functions as vectors.
Limiting procedure –



N equally spaced points, N+1 spaces of size

$$\Delta = x_{i+1} - x_i = \frac{L}{N+1}$$

$$x_0 = -\frac{L}{2},\ x_1 = -\frac{L}{2} + \Delta,\ \ldots,\ x_n = \frac{L}{2} - \Delta,\ x_{n+1} = \frac{L}{2}$$

ψ_i approximates $\psi(x)$

$$|\psi\rangle \doteq \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}$$

N dimensional vector space

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

inner product:

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

basis vectors are:

$$|x_i\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$ ← ith element is 1, all others are 0.

obviously

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

so

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

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

Hilbert space is limit $N \to \infty$. Inner product diverges, we should multiply by normalization factor $\Delta = \frac{L}{N+1}$

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

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

can easily extend to $L \to \infty$.

Completeness of basis,

$$I = \int dx \, |x\rangle\langle x|$$

$$\langle x_i | x_j \rangle = \delta_{ij} \xrightarrow{N \to \infty} \langle x' | x \rangle \equiv \delta(x' - x)$$

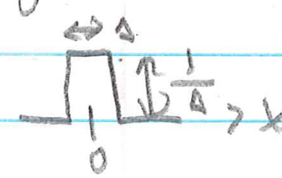
Kroenecker δ Dirac δ function

δ-function is not a function but a distribution, that is any function with limiting property

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

a, any interval containing $x = 0$.

Conceptually, unit area spike at $x = 0$,



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 show, $\delta(0) = \lim_{\lambda \to \infty} \frac{\lambda}{\pi} \to \infty$ diverge

and less easy but $\int_{-a}^{a} \delta(x)\, dx = \lim_{\lambda \to \infty} \frac{1}{\pi} \int_{-a}^{a} \frac{\sin \lambda x}{x} = 1$

lec 1-17

Properties:

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

2) derivative of step $\theta(x-a) = \begin{cases} 0 & x<a \\ 1 & x>a \end{cases}$

$$\frac{d\theta}{dx} = \delta(x-a)$$

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

4) derivative

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

and thus

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

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

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

integrate by parts, $f(|x|) \xrightarrow[x\to\infty]{} 0$

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

lec* -18

Derivative operator $\frac{d}{dx}$ is not Hermitian, but momentum operator $\frac{P_x}{\hbar} = \frac{1}{i}\frac{d}{dx} \equiv K_x$ is Hermitian

wave number op.

Need to show

$$\langle \phi | K_x \psi \rangle = \left(\langle K_x \psi | \phi \rangle\right)^* = \left(\langle \psi | K_x^+ \phi \rangle\right)^*$$

must equal $\left(\langle \psi | K_x \phi \rangle\right)^*$

work backwards,

$$\left(\langle \psi | K_x \phi \rangle\right)^* = \left(\int \psi^* \frac{1}{i}\frac{d}{dx} \phi \, dx\right)^*$$

integrate by parts

$$= \phi^* \frac{d\psi}{dx}\Big|_{-\infty}^{\infty} - \left(\int \phi \frac{\hbar}{i} \psi^* dx\right)^*$$

must go to 0 at $\pm\infty$

$$= + \int \phi^* \frac{\hbar}{i} \psi \, dx$$

$$= \langle \phi | K_x \psi \rangle \quad \checkmark$$

so operator $\frac{\hbar}{i}\frac{d}{dx} = P_x$ is Hermitian, $P_x^+ = P_x$ with real eigenvalues.