physics 491
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Lecture #4
Key points in Linear Algebra

Ref. Griffiths Ch 3., Shankar Ch 1.

Energy eigenstates form a basis in Hilbert space - a vector space of functions.

Euclidean Vectors

$\vec{r} \rightarrow (x, y, z)$ represented by.
$\vec{r} \cdot \vec{r} = (x^2+y^2+z^2)$ norm, invariant under rotations

Dirac Notation: $|a\rangle$ abstract vector

Linear Vector Space definition

① Addition rule $|c\rangle = |a\rangle + |b\rangle$
② scalar multiplication is distributive in vectors
③ " " " in scalars

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

③ scalar multiplication is associative

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

④ addition commutative $|v\rangle + |w\rangle = |w\rangle + |v\rangle$
⑤ addition is associative $|v\rangle + \big(|w\rangle + |x\rangle\big) = \big(|v\rangle + |w\rangle\big) + |x\rangle$

⑥ exists a null vector, $|0\rangle + |v\rangle = |v\rangle$

⑦ exists inverse under addition:

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

<u>Linear Independence</u>: Set of N vectors such that

any $|v\rangle = \sum_{i=1}^{N} c_i |i\rangle$ N is dimension of vector space.

$\{|i\rangle\}$ form a <u>basis</u>. and basis states are linearly independent.

ex. set of all 2×2 matrices form a vector space under matrix addition

$$|1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad |3\rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad |4\rangle = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

with complex scalars, a 4 dim'l complex vector space.

Components "represent" vector as column of numbers

$$|v\rangle \longrightarrow \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix}$$

Inner Product and Dual Space

For Euclidean vectors

$$\vec{A}\cdot\vec{B} = \underbrace{(A_x, A_y, A_z)}_{``\vec{A}\cdot"}\underbrace{\begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix}}_{\vec{B}}$$

"$\vec{A}\cdot$" maps vectors to scalars (numbers)

Generalize as linear maps on vector space

$$|V\rangle \xrightarrow{\langle w|} \text{scalar}$$ these maps also form a vector space called the dual space

Every vector has a dual

$$|v\rangle \rightarrow \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$$ "ket" has dual $\langle v| \rightarrow (v_1^*, \ldots, v_2^*)$ "bra"

the bracket is the inner product

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

① $\langle v|w\rangle = \langle w|v\rangle^*$

② $\langle v|v\rangle \geq 0$ equality iff $|v\rangle = |0\rangle$ null vector

③ $\langle v|\underbrace{(a|w\rangle + b|z\rangle)}_{\equiv |aw+bz\rangle} = a\langle v|w\rangle + b\langle v|z\rangle$

$\langle aw+bz|v\rangle = (\langle v|aw+bz\rangle)^* =$
$a^*\langle w|v\rangle + b^*\langle z|v\rangle$ anti-linear

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

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

Gram - Schmidt

Start w/ complete basis $\{|b_i\rangle\}$

$$|1\rangle \equiv \frac{|b_1\rangle}{\sqrt{\langle b_1|b_1\rangle}}$$ normalize one of them

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

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

Schwartz Inequality

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

triangle $\quad \big|\,|v\rangle + |w\rangle\big| \le \big||v\rangle\big| + \big||w\rangle\big|$

"norm" $\quad \big||v\rangle\big| \equiv \sqrt{\langle v|v\rangle}$

<u>Linear Operator</u>: linear map $|v\rangle \xrightarrow[\hat{T}]{} |v'\rangle$

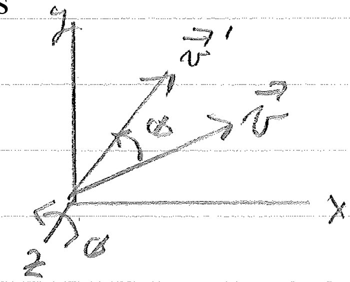
Use "Hat" to denote operator.

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

note: this is rotation of the vector, not change of basis

<u>Example</u>: rotation of Euclidean vector

$$\hat{R}^E_z \to \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



$$\hat{R}^E_y \hat{R}^E_z \neq \hat{R}^E_z \hat{R}^E_y$$

<u>rotations do not commute</u>

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

<u>Projection operator</u>: vector $|v\rangle$ in basis $\{|i\rangle\}$:

$$|v\rangle = \sum v_i |i\rangle$$

$$|v\rangle \to \begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix}$$

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

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

$$\hat{\mathbb{I}} = \sum |i\rangle\langle i|$$

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

In a basis, operators are represented by matrices.

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

$$\langle i|\hat{T}|v\rangle = \sum_j \langle i|\hat{T}|j\rangle\langle j|v\rangle$$

$$\begin{pmatrix} v_1' \\ \vdots \\ v_N' \end{pmatrix} = \begin{pmatrix} T_{ij} \end{pmatrix} \begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix}$$

row column.

$$\hat{T} \to [T_{ij}]$$

Transform of dual bra:

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

this defines the Hermitian conjugate

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

transpose

$$\hat{T}^\dagger \to (T_{ij}^*)^T$$

Hermitian conjugate

$$\boxed{T_{ij}^\dagger = T_{ji}^*}$$

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

one of the 3 Pauli spin matricies

if $\hat{T}^\dagger = \hat{T}$, T is Hermitian.

just as for any complex number,

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

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

H†=H A†=-A

Important: (easy to show that)

Eigenvalues of Hermitian matrix are real.

Observables correspond to Hermitian operators since measurements yield real numbers.

note that a unitary transformation preserves the norm.

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

Eigenvalue Problem

Given matrix $\hat{\Omega}$ find diagonal (N dim) basis $|\omega\rangle$

$$\hat{\Omega}|\omega\rangle = \omega|\omega\rangle$$

$|\omega\rangle$ ← eigenvector

ω ← eigenvalue

$$(\hat{\Omega} - \hat{I}\omega)|\omega\rangle = 0$$

Secular eq. $\det|\hat{\Omega} - \hat{I}\omega| = 0$ Nth order polynomial

Solve for eigenvalues ω_i.

for <u>each</u> ω_i, substitute back into eigenvalue equation to get components of $|\omega_i\rangle$ in non-diagonal basis.

$$|\omega_i\rangle \longrightarrow \begin{pmatrix} \omega_{1i} \\ \omega_{2i} \\ \vdots \\ \omega_{ni} \end{pmatrix}$$

One equation is redundant. Normalize $\langle\omega_i|\omega_i\rangle = 1$.
Matrix formed by eigenvectors as <u>columns</u> form diagonalization matrix

$$\hat{S} = \begin{pmatrix} \omega_{11} & \omega_{12} & \cdots \\ \omega_{21} & \vdots & \vdots \\ \vdots & & \end{pmatrix}$$ similarity matrix

$\hat{\Omega}' = \hat{S}^{+}\hat{\Omega}\hat{S}$ is diagonal.

Note that in this course we have used this definition of S which is the Hermitian conjugate of what I used in classical mechanics.

Diagonalization Example

Euclidean rotation $\hat{R}^E(\theta\hat{z}) = \begin{pmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{pmatrix}_{\theta=\pi/2} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$\hat{R}|u\rangle = \omega|u\rangle$

$(\hat{R} - \omega\hat{I})|u\rangle = 0$

$\det \begin{vmatrix} -\omega & -1 & 0 \\ 1 & -\omega & 0 \\ 0 & 0 & 1-\omega \end{vmatrix} = 0 = \omega^2(1-\omega) + (1-\omega) = 0$

$(\omega^2+1)(1-\omega) = 0$

$\omega = 1, i, -i$

$\underline{\omega = 1|}$ $\begin{pmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0$ $a = b = 0$, $c = 1$

$|1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

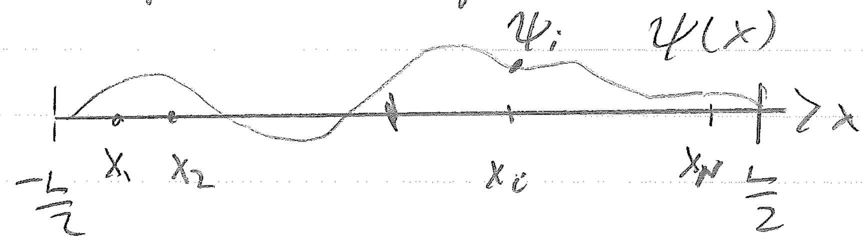
label by eigenvalue

$\underline{\omega = i|}$ $\begin{pmatrix} -i & -1 & 0 \\ 1 & -i & 0 \\ 0 & 0 & 1-i \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0$

$c = 0$ $\left.\begin{array}{l} -ia - b = 0 \\ a - ib = 0 \end{array}\right\}$ only 1 eq. $|i\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}$

$\underline{\omega = -i|}$ gives $|-i\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}$

<u>Hilbert space</u> An ∞ dimensional, non-denumerable vector space with functions as vectors



$\Delta \equiv x_{N+1} - x_N = \frac{L}{N+1}$ $\qquad x_i = -\frac{L}{2} + \frac{iL}{N}$

$\psi_i = \psi(x_i)$ approximates $\psi(x)$

$$|\psi\rangle \rightarrow \begin{pmatrix} \psi(x_1) \\ \vdots \\ \psi(x_N) \end{pmatrix}$$ form N dim linear vector space

$$|\psi\rangle + |\phi\rangle \rightarrow \begin{pmatrix} \psi(x_1) + \phi(x_1) \\ \vdots \\ \psi(x_N) + \phi(x_N) \end{pmatrix}$$

$$\langle \phi | \psi \rangle = \sum_i \phi^*(x_i)\,\psi(x_i)$$

basis vectors $|x_i\rangle \rightarrow \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$ i^{th} element 1

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

$$v(x_i) = \langle x_i | v \rangle$$

$$|v\rangle = \sum v(x_i)\,|x_i\rangle$$

In limit $N \to \infty$ our inner product diverges. We should multiply by suitable normalization factor

$$\Delta = \frac{L}{N+1}$$

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

$$\xrightarrow[N \to \infty]{} \int dx \, \phi^*(x) \, \psi(x)$$

$\langle x | \psi \rangle = \psi(x)$ amplitude to measure particle at position x.

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

must be careful about orthogonality

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

useful representation

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

plane wave states

$$\phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

orthogonal as $\int \phi_k^*(x)\, \phi_k(x')\, dk$

$$= \frac{1}{2\pi}\int e^{ik(x'-x)}\, dk = \delta(x'-x)$$

<u>and</u> $\int \phi_{k'}^*(x)\, \phi_k(x)\, dx = \frac{1}{2\pi}\int e^{i(k-k')x}\, dx$

$$= \delta(k-k')$$

Some properties of δ-function in appendix C

① Derivative of step is δ-function

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

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

② $$\delta(f(x)) = \frac{\delta(x-x_0)}{\left|\frac{df}{dx}\right|_{x=x_0}} \quad \text{where } f(x_0)=0$$

special case $\delta(ax) = \frac{1}{|a|}\delta(x)$

Fourier inversion

relate $\psi(x)$ to Fourier transform $\tilde{\psi}(k)$
where $k = \frac{p}{\hbar}$ "momentum space"

momentum space basis are plane wave states
(free particle energy eigenstates)

$$\phi_k(x) \equiv \frac{1}{\sqrt{2\pi}} e^{ikx}$$

$$\psi(x) = \int_{-\infty}^{\infty} \tilde{\psi}(k)\, \phi_k(x)\, dk$$

momentum space wave function
amplitude to have momentum $\hbar k$

then $\tilde{\psi}(k) = \int_{-\infty}^{\infty} \phi_k^*(x)\, \psi(x)\, dx$

Proof:

$$\psi(x) = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \phi_k^*(x')\, \psi(x')\, dx'\right] \phi_k(x)\, dk$$

exchange order of integration

$$\psi(x) = \int_{-\infty}^{\infty} dx' \, \psi(x') \left[\int_{-\infty}^{\infty} \phi_k^*(x') \, \phi_k(x) \, dk \right]$$

$$= \int_{-\infty}^{\infty} dx' \, \psi(x') \, \underbrace{\delta(x-x')}_{\delta(x'-x)} = \psi(x)$$

We can introduce the momentum basis $|k\rangle$ where

$$\langle x | k \rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} = \phi_k(x)$$

$$\langle k' | k \rangle = \delta(k'-k)$$

$$\int_{-\infty}^{\infty} |k\rangle\langle k| = \hat{1}$$

$$\psi(x) = \langle x | \psi \rangle = \int \langle x | k \rangle \langle k | \psi \rangle \, dk$$

$$= \int \phi_k(x) \, \tilde{\psi}(k) \, dk$$

so $\tilde{\psi}(k) = \langle k | \psi \rangle$ state vector $|\psi\rangle$ in $|k\rangle$ basis