# Optics & Spectroscopy — Lecture 12

## Dirac or "Bra-Ket" notation

$\hat{H}\Psi = E\Psi$ ~ eigenvalue equation

~ compare to linear algebra

$$\underbrace{\begin{pmatrix} a & b \\ c & d \end{pmatrix}}_{\text{matrix}} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = A \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

column vector

$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ ~ eigenvector of the matrix

$A$ ~ eigenvalue

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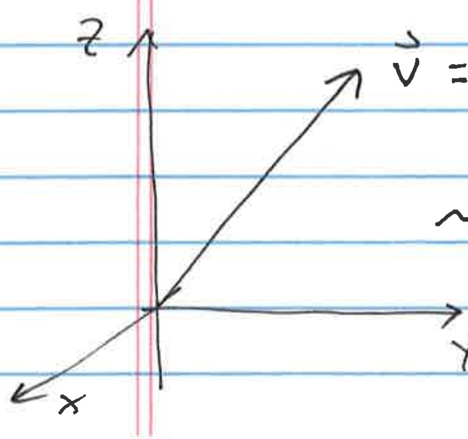
Some notes on vectors:




$\vec{V} = V_x\hat{x} + V_y\hat{y} + V_z\hat{z}$

~ represent as $(V_x, V_y, V_z)$

dot product: $\vec{u}\cdot\vec{v} = u_x v_x + u_y v_y + u_z v_z$

Matrix notation:

unit vectors $\hat{x} \equiv (1,0,0)$

$\hat{y} \equiv (0,1,0)$

$\hat{z} \equiv (0,0,1)$

dot product: $(u_x, u_y, u_z)\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = u_x v_x + u_y v_y + u_z v_z$

row vector
times column vector

~ any vector can be represented as a sum of unit vectors

$\vec{a} = \sum_{i=1}^{3} c_i \hat{e}_i$ $\quad \hat{e}_i$ ~ basis vectors

$\hat{e}_x \equiv \hat{x} \equiv (1\ 0\ 0)$ etc.

basis vectors are "orthonormal"

orthonormal

~ orthogonal $\hat{x} \cdot \hat{y} = (1\,0\,0)\begin{pmatrix}0\\1\\0\end{pmatrix} = 0$

~ normalized $\hat{x} \cdot \hat{x} = (1\,0\,0)\begin{pmatrix}1\\0\\0\end{pmatrix} = 1$

~ express this as: $\hat{e}_i \cdot \hat{e}_j = \delta_{ij}$

$$\delta_{ij} = 1 \quad i = j$$
$$= 0 \quad i \neq j$$

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In general, vector space can have any # of dimensions ~ could be infinite

i.e. $\vec{a} = \sum_{i=1}^{\infty} c_i \hat{e}_i$

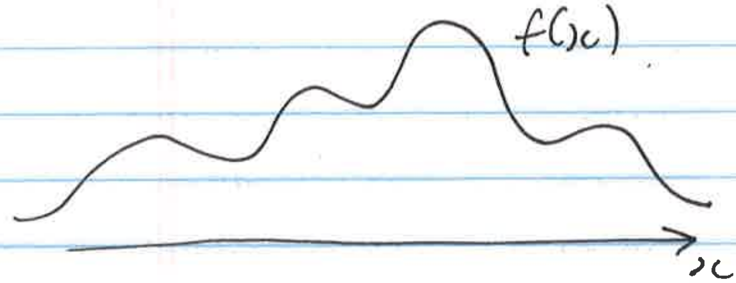
$$\hat{e}_5 = (0\,0\,0\,0\,1\,0\,0\,0 \ldots)$$

$\hat{e}_i$ ~ basis vectors

~ don't have to represent dimensions

~ could represent a set of functions

~ basis set consisting of functions is called "Hilbert Space"




← describe our function as a linear combination of functions

eg Hermite polynomials $H_n(x)$

Bessel function $J_n(x)$

eg. $f(x) = \sum_n c_n H_n(x) e^{-x^2/2}$

orthogonal: $\int_{-\infty}^{\infty} H_m(x) H_n(x) e^{-x^2} dx$

$= (\text{constant}) \times \delta_{nm}$

~ represent this sum as a row vector

$(c_1, c_2, c_3, c_4, \dots)$

infinite # of coefficients.

# Dirac Notation

$$\int \psi^* \hat{A} \psi \, d\vec{v} \equiv \langle \psi | \hat{A} | \psi \rangle$$

bra: $\langle \psi |$ ~ row vector

ket: $| \psi \rangle$ ~ column vector

operator: $\hat{A}$ ~ matrice

$$\langle \psi | \hat{A} | \psi \rangle \sim (\alpha \ \beta) \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \gamma \\ \delta \end{pmatrix}$$

Properties: $\hat{X}(|\alpha\rangle + |\beta\rangle) = \hat{X}|\alpha\rangle + \hat{X}|\beta\rangle$

$$\langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle^*$$

inner product

~ this is a number ( ≡ dot product of vectors )

$$\langle \alpha | \beta \rangle \equiv (a \ b) \begin{pmatrix} c \\ d \end{pmatrix} = ac + bd$$

~ we also have the outer product

$|\alpha\rangle\langle\beta|$ ~ matrix

eg $|\alpha\rangle\langle\beta| = \begin{pmatrix} a \\ b \end{pmatrix} (c \; d) = \begin{pmatrix} ac & ad \\ bc & bd \end{pmatrix}$

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Operators are like matrices:

associative $\hat{X}(\hat{Y}\hat{Z}) = (\hat{X}\hat{Y})\hat{Z}$

non-commutative $\hat{X}\hat{Y} \neq \hat{Y}\hat{X}$

eg $\hat{X}(\underbrace{\hat{Y}|\alpha\rangle}_{\text{do this } 1^{st}}) = (\underbrace{\hat{X}\hat{Y}}_{\text{multiply } 1^{st}})|\alpha\rangle \neq \hat{Y}(\hat{X}|\alpha\rangle)$

~ operators always operate on bra's from the right $(\langle\beta|\hat{X})$ and kets from the left $(\hat{X}|\alpha\rangle)$

~ products like $\hat{X}\langle\alpha|$ are illegal

cf. matrices $\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}$ ~ ok

$\begin{pmatrix} a \\ b \end{pmatrix}\begin{pmatrix} c & d \\ e & f \end{pmatrix}$ ~ no good

$(a\ b)\begin{pmatrix} c & d \\ e & f \end{pmatrix}$ ~ ok

Correspondence b/w bra & ket.

if $\hat{X}|\alpha\rangle = a|\alpha\rangle$ for ket $|\alpha\rangle$

then the corresponding equation for the bra

is: $\langle\alpha|\hat{X}^{+} = a^{*}\langle\alpha|$

$a^{*}$ ~ complex conjugate of $a$

$\hat{X}^{+}$ ~ "Hermitian adjoint" of $\hat{X}$

$\hat{X}$ ~ matrix

~ construct $\hat{X}^{+}$ by taking the c.c. of $\hat{X}$ and transposing

$$\Rightarrow (\hat{X}^+)_{ij} = (\hat{X}_{ji})^*$$

~ an operator is <u>Hermitian</u> if $\hat{X} = \hat{X}^+$

all observables in Q.M. are Hermitian

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~ consider a <u>Hermitian Operator</u> $\hat{A}$

eigenvectors: $|1\rangle, |2\rangle, |3\rangle, \ldots$

eigenvalues: $a_1, a_2, a_3, \ldots$

$$\Rightarrow \hat{A}|n\rangle = a_n|n\rangle$$

~ assume $|n\rangle$ are normalized $\Rightarrow \langle n|n\rangle = 1$

~ we also have

$$\langle n|\hat{A}^+ = a_n^* \langle n|$$

~ which is (for our Hermitian operator)

$$\langle n|\hat{A} = a_n \langle n|$$

Consider: $\hat{A}|n\rangle = a_n|n\rangle$

~ multiply b.s. by $\langle m|$ from the left

$$\langle m|\hat{A}|n\rangle = \langle m|a_n|n\rangle = a_n\langle m|n\rangle$$

now $\langle m|\hat{A} = a_m^*\langle m|$

$\Rightarrow \quad a_m^*\langle m|n\rangle = a_n\langle m|n\rangle$

$\Rightarrow \quad (a_m^* - a_n)\langle m|n\rangle = 0$

2 Cases: (i) $m=n$ $\quad (a_n^* - a_n)\langle n|n\rangle = 0$

$$\langle n|n\rangle = 1$$

$$\Rightarrow a_n^* = a_n$$

~ this means the eigenvalues of Hermitian Operators are real

~ operators that correspond to observables are Hermitian (only measure real #s)

(ii) $m \neq n$ now $(a_m^* - a_n) = 0$

$\Rightarrow \langle m | n \rangle = 0$

~ eigenvectors of Hermitian operators are orthogonal

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Hamiltonian is Hermitian (energy is an observable)

$H | n \rangle = E_n | n \rangle$

~ eigenvectors have real eigenvalues ($E_n$'s) and they are orthogonal

~ use the eigenvectors as a "basis set" for writing down a general wavefunction

$| \psi \rangle = \sum_n c_n | n \rangle$

$$|\psi\rangle = \sum_n c_n |n\rangle$$

~ multiply from the left by $\langle j|$

$$\langle j|\psi\rangle = \langle j| \sum_n c_n |n\rangle$$

$$= \sum_n c_n \langle j|n\rangle$$

$|n\rangle$ ~ orthogonal $\Rightarrow$ $\langle j|n\rangle = \delta_{jn}$

$$\langle j|n\rangle = 0 \quad j \neq n$$
$$= 1 \quad j = n$$

~ only term that survives in the sum is the term $n = j$

$$\Rightarrow \langle j|\psi\rangle = c_j$$

Go back to $|\psi\rangle = \sum_n c_n |n\rangle$

rewrite : $|\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle$

↖ just a #

$$|\psi\rangle = \sum_n c_n |n\rangle = \sum_n |n\rangle c_n$$

doesn't matter where we put $c_n$

$$\Rightarrow |\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle$$

$$= \sum_n |n\rangle\langle n|\psi\rangle$$

$$\Rightarrow \sum_n |n\rangle\langle n| = 1$$ ~ closure relationship

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$$\langle\psi|\psi\rangle = \langle\psi|\sum_n |n\rangle\langle n|\psi\rangle$$

$$= \sum_n \underbrace{\langle\psi|n\rangle}_{c_n^*}\underbrace{\langle n|\psi\rangle}_{c_n} = \sum_n |c_n|^2$$

$|\psi\rangle$ is normalized if $\langle\psi|\psi\rangle = \sum_n |c_n|^2 = 1$

Back to the start of the lecture:

Bra-ket notation

$$\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle \quad \left( \equiv \int \psi^* \hat{H} \psi \, d\vec{v} \right)$$

$$|\psi\rangle = \sum_n c_n |n\rangle$$

$$\Rightarrow \langle E \rangle = \langle \psi | \hat{H} \sum_n c_n |n\rangle$$

$$= \langle \psi | \sum_n c_n \hat{H} |n\rangle = \langle \psi | \sum_n c_n E_n |n\rangle$$

now, $\langle \psi | = \sum_m c_m^* \langle m |$

$$\Rightarrow \langle E \rangle = \sum_m \sum_n c_m^* \langle m | c_n E_n | n \rangle$$

$$= \sum_m \sum_n c_m^* c_n E_n \underbrace{\langle m | n \rangle}_{\delta_{mn}}$$

$$= \sum_n |c_n|^2 E_n$$

$|c_n|^2 \sim$ prob of finding the state "$n$" in our wavefunction