Analogy between functions and vectors allows us to turn QM into linear algebra by a systematic procedure

- To solve QM on computers

Vectors		Functions		Brackets	
vector	$\vec{v}$	Function	$\psi(x)$	ket	$\lvert\psi\rangle$
basis vector	$\vec{w}_n$	basis function	$\varphi_n(x)$	basis set	$\lvert n\rangle$
vector dot prod	$\vec{w}^{+}_{m}\cdot$	overlap integral	$\int dx\, \varphi_m^*(x)$	bra	$\langle m\rvert$
matrix	$\underset{\approx}{A}$				

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The analogy is possible because of a Theorem from 265

- Solution $\varphi_n(x)$ of eigenvalue differential eqn. $\hat{A}\varphi_n(x) = a_n\varphi_n(x)$ form a complete ortho-normal basis:

Vector	Function	Ket	
$\vec{w}_n^{+}\cdot\vec{w}_n = 1$	$\int dx\, \varphi_n^* \varphi_n(x) = 1$	$\langle n\lvert n\rangle = 1$	normalized
$w_n^{+}\cdot\vec{w}_m = 0$	$\int dx\, \psi_n^{+}\varphi_m(x) = 0$	$\langle n\lvert m\rangle = 0$	orthogonal
$\vec{v} = \sum_n c_n \vec{w}_n$	$\psi(x) = \sum c_n \varphi_n(x)$	$\lvert\psi\rangle = \sum_n \langle n\lvert n)$	complete basis

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what does "$+\cdot$" mean

complex conjugate transpose dot product

$$\vec{v} = \frac{1}{\sqrt{2}}\vec{u}_1 + \frac{i}{\sqrt{2}}\vec{w}_2 = \vec{v} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{i}{\sqrt{2}}\begin{pmatrix}0\\i\end{pmatrix} = \begin{pmatrix}1/\sqrt{2}\\ i/\sqrt{2}\end{pmatrix}$$

$$\vec{v}^{+}\cdot = \left(1/\sqrt{2} \;\; -i\, 1/\sqrt{2}\right)\cdot \Rightarrow \vec{v}^{+}\cdot v = \left(1/\sqrt{2} \;\; -i/\sqrt{2}\right)\begin{pmatrix}1/\sqrt{2}\\ i/\sqrt{2}\end{pmatrix} = \frac{1}{2} + \frac{1}{2} = 1$$

resulting vector is normalized

In bracket notation $\lvert v\rangle = \frac{1}{\sqrt{2}}\lvert 1\rangle + \frac{i}{\sqrt{2}}\lvert 2\rangle$

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Given basis vectors $\vec{w}_n$ and vector $\vec{v}$, how do you get c_n?

$$\vec{v} = \sum c_n \vec{w}_n$$

$$\vec{w}_m^{+}\cdot\vec{v} = \sum c_n \vec{w}_m^{+}\cdot\vec{w}_n \;(= 0 \text{ if } m \neq n)$$

Function analogy $\psi(x) = \sum_n c_n \varphi_n(x) \Rightarrow c_n = \int dx\, \varphi_m^*(x)\psi(x)$

Bracket analogy: $\lvert\psi\rangle = \sum_n c_n\lvert n\rangle \Rightarrow c_m = \langle m\lvert\psi\rangle$

Consider a special case of interest

$\hat{A} = \hat{H}$; $\chi(x) = E\psi(x)$; $\varphi_n(x)$ any complete basis (e.g. he)

Then $\hat{A}\psi = \chi \Rightarrow \quad \hat{H}\psi = E\psi \quad \left\{ \begin{array}{l} H_{nm} = \int dx\, \psi_m^* H \varphi_n \\ \vec{v} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} \psi(x) = \sum_n c_n \varphi_n \end{array} \right.$

$\hat{=} \quad \underset{\approx}{\hat{H}}\vec{v} = E\vec{v}$

$\hat{=} \quad \underset{\approx}{H}\vec{v} = E\underset{\approx}{I}\vec{v}$

$$\hat{=} \begin{pmatrix} H_{11} & H_{12} & \cdots \\ H_{21} & H_{22} & \\ \vdots & & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \begin{pmatrix} E & 0 & 0 & \cdots \\ 0 & E & 0 & \\ 0 & 0 & E & \\ \vdots & & & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} \begin{array}{l} \leftarrow \varphi_1(x) \\ \leftarrow \varphi_2(x) \\ \vdots \end{array} \Bigg\} \psi(x)$$

Allows you to calculate the eigenfunctions of ANY hamiltonian using any basis set that covers the same coordinates

$\Rightarrow (\underset{\approx}{H} - E\underset{\approx}{I}) \cdot \vec{v} = 0$ has a solution only if

$\det |\underset{\approx}{H} - E\underset{\approx}{I}| = 0$

$$\begin{vmatrix} H_{11} - E & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} - E & H_{23} & \\ \vdots & \vdots & & \ddots \\ \vdots & \vdots & & \end{vmatrix} = 0 \Rightarrow n^{th} \text{ order poly in } E$$

$\Rightarrow n$ values of E

$\Rightarrow n$ vectors $\vec{v}$

$\Rightarrow n$ functions $\psi(x)$