Matrix Formulation of QM

complete orthonormal set

$$|\psi\rangle = \sum_n c_n |n\rangle , \quad |\psi\rangle \to \{c_n\} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \\ \vdots \end{pmatrix}$$

$$|u_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \qquad |u_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$$

$$|\psi\rangle = \sum_n c_n |u_n\rangle \to \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} = c_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$$

If ket's are represented by column vectors, then bra's are represented by the transpose conjugate of column = row, complex conjugate

$$|\psi\rangle = \sum_n c_n |u_n\rangle \longrightarrow \langle\psi| = \sum_n c_n^* \langle u_n|$$

$$\langle\psi| = \begin{pmatrix} c_1^* & c_2^* & c_3^* & \dots \end{pmatrix}$$

$$\langle\psi|\psi\rangle = \begin{pmatrix} c_1^* & c_2^* & c_3^* & \dots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} = |c_1|^2 + |c_2|^2 + \dots = \sum_n |c_n|^2$$

Operators can be represented by matrices:

no hat on matrix element

$$\hat{A} \longrightarrow \{A_{mn}\} = \{\langle m|\hat{A} n\rangle\} = \begin{pmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \\ \vdots & & \end{pmatrix}$$

where $\{|n\rangle\}$ is some complete orthonormal set

where from?

$\partial,$

Consider the operator $\hat{A}$ and 2 state vectors $|\Psi\rangle, |\varphi\rangle$ related by

$$|\varphi\rangle = \hat{A}|\Psi\rangle \qquad (\star)$$

in basis $\{|n\rangle\}$, $|\Psi\rangle = \sum_n c_n|n\rangle = \sum_n |n\rangle\underbrace{\langle n|\Psi\rangle}_{c_n}$

$$|\varphi\rangle = \sum_n d_n|n\rangle = \sum_n |n\rangle\underbrace{\langle n|\varphi\rangle}_{d_n}$$

Now project eq'n $\star$ onto $|m\rangle$ by acting w/ bra:

$$\langle m|\varphi\rangle = \langle m|\hat{A}|\Psi\rangle = \sum_n c_n \langle m|\hat{A}|n\rangle$$

$$d_n = \sum_n A_{mn}\, c_n$$

This is the rule for multiplication of Matrix $\times$ column

$$\begin{pmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \\ \vdots & & \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$$

Suppose $\hat{A} = \hat{H}$ and $\{|n\rangle\}$ are energy eigenstates, then

$$\hat{H}|n\rangle = E_n|n\rangle, \quad H_{mn} = \langle m|\hat{H}|n\rangle = E_n\,\delta_{mn}$$

$$\hat{H}|2\rangle = E_2|2\rangle \Rightarrow \begin{pmatrix} E_1 & & & 0 \\ & E_2 & & \\ & & E_3 & \\ 0 & & & \ddots \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} = E_2\begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$$

A matrix operator $\langle m|\hat{A}|n\rangle$ is <u>diagonal</u> when represented in the basis of its own eigenstates, and the diagonal elements are the eigenvalues

Notice that in <u>general</u> operators don't commute $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

Same goes for Matrix Multiplication: $\mathbb{A}\mathbb{B} \neq \mathbb{B}\mathbb{A}$

Claim: The matrix of a hermitian operator is equal to its transpose conjugate:

$$\boxed{\hat{A} \text{ hermitian} \Leftrightarrow A_{mn} = A^*_{nm}}$$

Proof: $\langle m|\hat{A}n\rangle = \langle \hat{A}m|n\rangle = \langle n|\hat{A}m\rangle^*$

$$\Rightarrow A_{mn} = A^*_{nm}$$

Similarly, adjoint $\hat{A}^+$: $A^+_{mn} = A^*_{nm}$

Proof: $\langle \hat{A}m|n\rangle = \langle m|\hat{A}^+n\rangle = \langle n|\hat{A}m\rangle^*$

Of course, it difficult to do calculations if the matrices and columns are infinite dimensional. But there are Hilbert <u>subspaces</u> that are finite dimensional. For instance, in the H-atom, the full space of bound states is spanned by the full set $\{n, l, m\}$ $(=|nlm\rangle)$. The sub-set $\{n=2, l=1, m=+1, 0, -1\}$ forms a vector space called a <u>subspace</u>.

Subspace? In ordinary Euclidean space, any plane is a subspace of the full volumn. If we consider just the xy components of a vector

$$\vec{R}_{xy} = \hat{x}R_x + \hat{y}R_y$$, then we have a

perfectly valid 2D vector space, even though the "true" vector is 3D.

Likewise, in Hilbert space, we can restrict our attention to a subspace spanned by a small nbr of basis states.

Example: H-atom subspace $\{n=2, l=1, m=1,0,-1\}$

Basis states are $\{|m\rangle\} = |+1\rangle, |0\rangle, |-1\rangle$
(can drop $n=2$, $l=1$ in label since they are fixed.)

$$\hat{L}_z |m\rangle = \hbar m |m\rangle$$

$$\hat{L}^2 |m\rangle = \hbar^2 l(l+1)|m\rangle \overset{(l=1)}{=} 2\hbar^2 |m\rangle \quad \text{(for all } m\text{)}$$

$$\Rightarrow \quad (L_z)_{mn} = \langle m|\hat{L}_z|n\rangle = \hbar \begin{pmatrix} +1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$L^2_{mn} = \langle m|\hat{L}^2|n\rangle = 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

What about L_x? L_y?

Before seeing what all this ~~spin~~ matrix stuff is good for, let's examine spin because it's very important physically and because it will lead to 2D Hilbert space with simple 2×2 matrices.