Hilbert Space and Dirac notation

- An (in)finite-dimensional vector (or function) space of square-integrable vectors (or functions)

- Vectors (or functions) are denoted by "Kets" $|f\rangle$

- Inner product of $|f\rangle$ with $|g\rangle$ is obtained by taking Hermitian conjugate + multiplying $|f\rangle^{\dagger}|g\rangle$

- There is also a dual Hermitian-conjugate Hilbert space of "bras" $\langle g|$. Inner products can therefore be written

$$|f\rangle^{\dagger}|g\rangle = \langle f|g\rangle$$

This works for finite-dimensional vectors, <u>or</u> functions eg. functions of x:

$$\langle f|g\rangle = \int_{-\infty}^{\infty} f^{*}(x)\, g(x)\, dx$$

- $\langle f|f\rangle$ is real and non-negative
- orthonormal basis set $|f_n\rangle$ $n=1,2,3\ldots$

$$\langle f_n|f_m\rangle = \delta_{nm}$$

- basis set is complete if any vector (or function) in Hilbert space can be expressed as a linear combination of basis vectors (or functions)

$$|f\rangle = \sum_n c_n |f_n\rangle$$

Then, $\langle f_m|f\rangle = \sum_n c_n \langle f_m|f_n\rangle = \sum_n c_n \delta_{nm} = c_m$

So $c_n = \langle f_n|f\rangle$

Note:

$$|f\rangle = \sum_n |f_n\rangle\langle f_n|f\rangle = \left(\sum_n |f_n\rangle\langle f_n|\right)|f\rangle$$

$$\sum_n |f_n\rangle\langle f_n| = \hat{1} \quad \text{(identity)}$$

Observables are Hermitian operators

- They have real eigenvalues and orthonormal eigenvectors (or eigenfunctions)
- Commute w/ vectors in Hilbert space

$$\langle f|Q|f\rangle = \langle f|Qf\rangle = (\langle f|Qf\rangle)^{\dagger} = \langle Q^{\dagger}f|f\rangle = \langle Qf|f\rangle$$

- The matrix elements of Q in the $|f_n\rangle$ basis are

$$\langle f_n|Q|f_m\rangle$$

Example: $Q = H \longrightarrow \langle \varphi_m|H|\varphi_n\rangle = \langle \varphi_m|E_n|\varphi_n\rangle = E_n\langle \varphi_m|\varphi_n\rangle = E_n\,\delta_{mn}$

$$\begin{bmatrix} E_1 & 0 & 0 & 0 & \cdots \\ 0 & E_2 & 0 & - & \\ 0 & 0 & E_3 & & \\ \vdots & \vdots & & \ddots & \end{bmatrix}$$

(a diagonal matrix)

$\rightarrow$ The eigenfunctions/vectors of an operator "diagonalize" that operator!

Example

$$\hat{H} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \left(\text{in basis } |X\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } |Y\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right)$$

1. Show that $\langle n | \hat{H} | m \rangle$ is the n^{th} row, m^{th} column element of H:

$$H_{11} = \langle X | H | X \rangle = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0, \quad H_{12} = \langle X | H | Y \rangle = H^{\dagger}_{21} = 1$$

$$H_{21} = \langle Y | H | X \rangle = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 1, \quad H_{22} = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0$$

2. What are the eigenvalues of $\hat{H}$?

$$\hat{H} |\Psi\rangle = E |\Psi\rangle \quad \text{(Schrödinger equation)}$$

$$(\hat{H} - E\hat{I}) |\Psi\rangle = 0$$

$$\det \begin{bmatrix} -E & 1 \\ 1 & -E \end{bmatrix} = 0$$

$$E^2 - 1 = 0$$

$$E = \pm 1$$

$$E_+ = +1, \quad E_- = -1$$

3. What are the eigenvectors of $\hat{A}$?

$$(\hat{A} - E_+ \hat{I})|+\rangle = 0$$

$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 0$$

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$(\hat{A} - E_- \hat{I})|-\rangle = 0$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 0$$

$$|-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

4. Show that $\sum_n |\varphi_n\rangle\langle\varphi_n| = \hat{I}$

$$|+\rangle\langle+| + |-\rangle\langle-|$$

$$\frac{1}{2}\left(\begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \end{bmatrix} + \begin{bmatrix} 1 \\ -1 \end{bmatrix} \begin{bmatrix} 1 & -1 \end{bmatrix} \right) = \frac{1}{2}\left(\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \right) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \hat{1} \checkmark$$

Octave

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octave-3.2.2.exe:7:~\Desktop\PHYS401\code
> bra_ket(4)
A random complex-valued Hermitian matrix:
H =

   0.53427 + 0.00000i   1.55496 - 0.48363i   0.98593 + 0.41434i   1.04617 - 0.08737i
   1.55496 + 0.48363i   1.17180 + 0.00000i   0.69207 - 0.14460i   1.38173 + 0.10256i
   0.98593 - 0.41434i   0.69207 + 0.14460i   0.12701 + 0.00000i   1.28715 + 0.40134i
   1.04617 + 0.08737i   1.38173 - 0.10256i   1.28715 - 0.40134i   1.66651 + 0.00000i

Notice that the outer product (column vector times row vector) of eigenvectors is a matrix:
ans =

   0.41404 + 0.00000i  -0.23109 + 0.10564i  -0.25090 - 0.30816i   0.03233 + 0.13815i
  -0.23109 - 0.10564i   0.15593 + 0.00000i   0.06141 + 0.23601i   0.01720 - 0.08536i
  -0.25090 + 0.30816i   0.06141 - 0.23601i   0.38141 + 0.00000i  -0.12242 - 0.05965i
   0.03233 - 0.13815i   0.01720 + 0.08536i  -0.12242 + 0.05965i   0.04862 + 0.00000i

when we sum the outer products of eigenvectors, we get the identity to within machine precision
C =

   1.00000 + 0.00000i   0.00000 + 0.00000i   0.00000 - 0.00000i  -0.00000 - 0.00000i
   0.00000 - 0.00000i   1.00000 + 0.00000i   0.00000 - 0.00000i  -0.00000 + 0.00000i
   0.00000 + 0.00000i   0.00000 + 0.00000i   1.00000 + 0.00000i  -0.00000 - 0.00000i
  -0.00000 + 0.00000i  -0.00000 - 0.00000i  -0.00000 + 0.00000i   1.00000 + 0.00000i

the maximum error for the elements of this random matrix is:
1.3878e-016 + 2.0817e-016i
whereas machine precision on this computer is 2.2204e-016
octave-3.2.2.exe:8:~\Desktop\PHYS401\code
>
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