Hermitian Operators

- Definition: an operator is said to be Hermitian if it satisfies: $A^{\dagger}=A$
  - Alternatively called 'self adjoint'
  - In QM we will see that all observable properties must be represented by Hermitian operators

- Theorem: all eigenvalues of a Hermitian operator are real
  - Proof:
    - Start from Eigenvalue Eq.: $A|a_m\rangle = a_m|a_m\rangle$
    - Take the H.c. (of both sides): $\langle a_m|A^{\dagger} = a_m^*\langle a_m|$
    - Use $A^{\dagger}=A$: $\langle a_m|A = a_m^*\langle a_m|$
    - Combine to give:
      $$\langle a_m|A|a_m\rangle = a_m^*\langle a_m|a_m\rangle = a_m\langle a_m|a_m\rangle$$
    - Since $\langle a_m|a_m\rangle \neq 0$ it follows that
      $$a_m^* = a_m$$

Eigenvectors of a Hermitian operator

- Note: all eigenvectors are defined only up to a multiplicative c-number constant
  $$A|a_m\rangle = a_m|a_m\rangle \quad \to A\left(c|a_m\rangle\right) = a_m\left(c|a_m\rangle\right)$$
  - Thus we can choose the normalization $\langle a_m|a_m\rangle=1$

- THEOREM: all eigenvectors corresponding to distinct eigenvalues are orthogonal
  - Proof:
    - Start from eigenvalue equation: $A|a_m\rangle = a_m|a_m\rangle$
    - Take H.c. with m $\to$ n: $\langle a_n|A = a_n\langle a_n|$
    - Combine to give:
      $$\langle a_n|A|a_m\rangle = a_n\langle a_n|a_m\rangle = a_m\langle a_n|a_m\rangle$$
    - This can be written as: $(a_n - a_m)\langle a_n|a_m\rangle = 0$
    - So either $a_m = a_n$ in which case they are not distinct, or $\langle a_m|a_n\rangle=0$, which means the eigenvectors are orthogonal

Completeness of Eigenvectors of a Hermitian operator

- THEOREM: If an operator in an M-dimensional Hilbert space has M distinct eigenvalues (i.e. no degeneracy), then its eigenvectors form a `complete set' of unit vectors (i.e a complete 'basis')
  - Proof:

    M orthonormal vectors must span an M-dimensional space.

- Thus we can use them to form a representation of the identity operator:

Degeneracy

- Definition: If there are at least two linearly independent eigenvectors associated with the same eigenvalue, then the eigenvalue is degenerate.
  - The `degree of degeneracy' of an eigenvalue is the number of linearly independent eigenvectors that are associated with it
    - Let d_m be the degeneracy of the m^{th} eigenvalue
    - Then d_m is the dimension of the degenerate subspace

- Example: The d=2 case
  - Let's refer to the two linearly independent eigenvectors $|\omega_n\rangle$ and $|\Omega_n\rangle$
    - There is some operator W such that for some n we have:

      $W|\omega_n\rangle = \omega_n|\omega_n\rangle$ and $W|\Omega_n\rangle = \Omega_n|\Omega_n\rangle$
    - Also we choose to normalize these states:

      $\langle\omega_n|\omega_n\rangle=1$ and $\langle\Omega_n|\Omega_n\rangle=1$
    - Linear independence means $\langle\omega_n|\Omega_n\rangle \neq 1$.

  - If they are not orthogonal ($\langle\omega_n|\Omega_n\rangle \neq 0$), we can always use Gram-Schmidt Orthogonalization to get an orthonormal set

Gram-Schmidt Orthogonalization

- Procedure:
  - Let $$|\omega_n,1\rangle \equiv |\omega_n\rangle$$
  - A second orthogonal vector is then

$$|\omega_n,2\rangle \equiv \frac{|\Omega_n\rangle - |\omega_n\rangle\langle\omega_n|\Omega_n\rangle}{\left\| |\Omega_n\rangle - |\omega_n\rangle\langle\omega_n|\Omega_n\rangle \right\|}$$

    - Proof:

$$\langle\omega_n,1|\omega_n,2\rangle \equiv \frac{\langle\omega_n|\Omega_n\rangle - \langle\omega_n|\omega_n\rangle\langle\omega_n|\Omega_n\rangle}{\left\| |\Omega_n\rangle - |\omega_n\rangle\langle\omega_n|\Omega_n\rangle \right\|}$$

      - but $\langle\omega_n|\omega_n\rangle = 1$
      - Therefore $\langle\omega_n,1|\omega_n,2\rangle = 0$
  - Can be continued for higher degree of degeneracy
  - Analogy in 3-d:

$$\vec{r} = \vec{e}_x r_x + \vec{e}_y r_y + \vec{e}_z r_z$$

$$\vec{r} = \vec{e}_x(\vec{e}_x \cdot \vec{r}) + \vec{e}_y(\vec{e}_y \cdot \vec{r}) + \vec{e}_z(\vec{e}_z \cdot \vec{r})$$

$$\vec{r} - \vec{e}_x(\vec{e}_x \cdot \vec{r}) \perp \vec{e}_x \qquad |r\rangle - |e_x\rangle\langle e_x|r\rangle \perp |e_x\rangle$$

- Result: From M linearly independent degenerate eigenvectors we can always form M orthonormal unit vectors which span the M-dimensional degenerate subspace.
  - If this is done, then the eigenvectors of a Hermitian operator form a complete basis even with degeneracy present

Phy851/Lecture 4: Basis sets and representations

- A \`basis' is a set of orthogonal unit vectors in Hilbert space
  - analogous to choosing a coordinate system in 3D space
  - A basis is a complete set of unit vectors that spans the state space

- Basis sets come in two flavors: ‘discrete’ and ‘continuous’

  - A discrete basis is what we have been considering so far. The unit vectors can be labeled by integers, e.g. $\{|1\rangle, |2\rangle, \ldots, |M\rangle\}$, where M can be either finite <u>or infinite</u>
    - The number of basis vectors is either finite or ‘countable infinity’.

  - A continuous basis is a generalization whereby the unit vectors are labeled by real numbers, e.g. $\{|x\rangle\}$; $x_{\min} < x < x_{\max}$, where the upper and lower bounds can be either finite or infinite
    - The number of basis vectors is \`uncountable infinity'.

Properties of basis vectors

property	discrete	continuous
orthogonality	$\langle j \| k\rangle = \delta_{jk}$	$\langle x \| x'\rangle = \delta(x - x')$
normalization	$\langle j \| j\rangle = 1$	$\langle x \| x\rangle = \infty$
state expansion	$\|\psi\rangle = \sum_j \|j\rangle c_j$	$\|\psi\rangle = \int dx \|x\rangle \psi(x)$
component/ wavefunction	$c_j \equiv \langle j \| \psi\rangle$	$\psi(x) \equiv \langle x \| \psi\rangle$
projector	$1 = \sum_j \|j\rangle\langle j\|$	$1 = \int dx \|x\rangle\langle x\|$
operator expansion	$A = \sum_{jk} \|j\rangle A_{jk} \langle k\|$	$A = \int dx dx' \|x\rangle A(x,x')\langle x'\|$
Matrix element	$A_{jk} \equiv \langle j \| A \| k\rangle$	$A(x,x') \equiv \langle x \| A \| x'\rangle$

$$1^2 = 1$$

$$\begin{aligned}\left[\int dx|x\rangle\langle x|\right]^2 &= \int dx\, dx' |x\rangle\langle x|x'\rangle\langle x'| \\ &= \int dx\, dx' |x\rangle \delta(x - x')\langle x'| \\ &= \int dx |x\rangle\langle x|\end{aligned}$$

Example 1

- Consider the relation: $|\psi'\rangle = A|\psi\rangle$
  - To know $|\psi\_\rangle$ or $|\psi\rangle$ you must know its components in some basis
  - Here we will go from the abstract form to the specific relation between components

Abstract equation: $|\psi'\rangle = A|\psi\rangle$

Project onto a single unit vector: $\langle j|\psi'\rangle = \langle j|A|\psi\rangle$

Insert the projector: $\langle j|\psi'\rangle = \sum_k \langle j|A|k\rangle\langle k|\psi\rangle$

Translate to vector notation: $c'_j = \sum_k A_{jk} c_k$

Same procedure for continuous basis:

$$|\psi'\rangle = A|\psi\rangle$$

$$\langle x|\psi'\rangle = \langle x|A|\psi\rangle$$

$$\langle x|\psi'\rangle = \int dx' \langle x|A|x'\rangle\langle x'|\psi\rangle$$

$$\psi'(x) = \int dx' A(x,x')\psi(x')$$

Example 2: Combining different basis sets in a single expression

- Let's assume we know the components of $|\varphi\rangle$ in the basis $\{|1\rangle,|2\rangle,|3\rangle,\ldots\}$
  - $c_j \equiv \langle j|\varphi\rangle$
- Let's suppose that we only know the wavefunction of $|\psi\rangle$ in the continuous basis $\{|x\rangle\}$
  - $\psi(\mathrm{x}) \equiv \langle \mathrm{x}|\psi\rangle$
- In addition, we only know the matrix elements of A in the alternate continuous basis $\{|k\rangle\}$
  - $A(k,k') \equiv \langle k|\mathrm{A}|\mathrm{k}'\rangle$
- How would we compute the matrix element $\langle\varphi|A|\psi\rangle$?

$$
\begin{aligned}
\langle\varphi|A|\psi\rangle &= \langle\varphi|A|\psi\rangle \\
&= \sum_j \langle\varphi|j\rangle\langle j|A|\psi\rangle \\
&= \sum_j \int dx \langle\varphi|j\rangle\langle j|A|x\rangle\langle x|\psi\rangle \\
&= \sum_j \int dx\,dk\,dk' \langle\varphi|j\rangle\langle j|k\rangle\langle k|A|k'\rangle\langle k'|x\rangle\langle x|\psi\rangle \\
&= \sum_j \int dx\,dk\,dk'\, c_j^* \langle j|k\rangle A(k,k')\langle k'|x\rangle\psi(x)
\end{aligned}
$$

- We see that in order to compute this number, we need the inner-products $\langle j|k\rangle$ and $\langle k|\psi\rangle$
  - These are the transformation coefficients to go from one basis to another

Change of Basis

- Let the sets $\{|1\rangle,|2\rangle,|3\rangle,\ldots\}$ and $\{|u_1\rangle,|u_2\rangle,|u_3\rangle,\ldots\}$ be two different orthonormal basis sets
- Suppose we know the components of $|\psi\rangle$ in the basis $\{|1\rangle,|2\rangle,|3\rangle,\ldots\}$, this means we know the elements $\{c_j\}$:
- How do we find the components $\{C_j\}$ of $|\psi\rangle$ in the alternate basis $\{|\mathrm{u}_1\rangle,|\mathrm{u}_2\rangle,|\mathrm{u}_3\rangle,\ldots\}$
- This is easily handled with Dirac notation:

$$
\begin{aligned}
\langle\varphi|A|\psi\rangle &= \sum_j \langle\varphi|j\rangle\langle j|A|\psi\rangle \\
&= \sum_j \int dx \langle\varphi|j\rangle\langle j|A|x\rangle\langle x|\psi\rangle \\
&= \sum_j \int dx\,dk\,dk' \langle\varphi|j\rangle\langle j|k\rangle\langle k|A|k'\rangle\langle k'|x\rangle\langle x|\psi\rangle \\
&= \sum_j \int dx\,dk\,dk'\, c_j^* \langle j|k\rangle A(k,k')\langle k'|x\rangle\psi(x)
\end{aligned}
$$

- The change of basis is accomplished by multiplying the original column vector by a transformation matrix U.

The Transformation matrix

- The transformation matrix looks like this

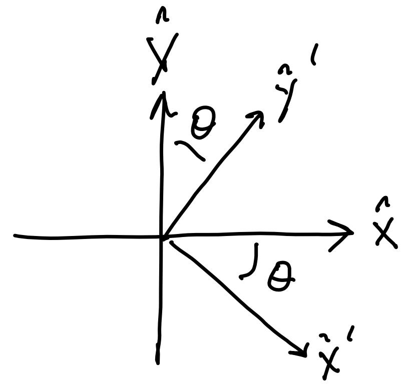
$$U = \begin{pmatrix} \langle u_1|1\rangle & \langle u_1|2\rangle & \langle u_1|3\rangle & \cdots \\ \langle u_2|1\rangle & \langle u_2|2\rangle & \langle u_2|3\rangle & \cdots \\ \langle u_3|1\rangle & \langle u_3|2\rangle & \langle u_3|3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

- The columns of U are the components of the old unit vectors in the new basis

- If we specify at least one basis set in physical terms, then we can define other basis sets by specifying the elements of the transformation matrix

Example: 2-D rotation

- Let's do a familiar problem using the new notation
- Consider a clockwise rotation of 2-dimensional Cartesian coordinates:



$$\vec{r} = r_x \hat{x} + r_y \hat{y}$$

$$\vec{r} = r'_x \hat{x}' + r'_y \hat{y}'$$

$$\downarrow$$

$$|r\rangle = |\hat{x}\rangle r_x + |\hat{y}\rangle r_y$$

$$= |\hat{x}'\rangle r'_y + |\hat{y}'\rangle r'_y$$

$$\hat{x}'\cdot\hat{x} = \cos\theta$$

$$\hat{x}'\cdot\hat{y} = -\sin\theta$$

$$\hat{y}'\cdot\hat{x} = \sin\theta$$

$$\hat{y}'\cdot\hat{y} = \cos\theta$$

$r_x, r_y \rightarrow$ known

$r'_x, r'_y \rightarrow$ unknown

Continued

- FIND r'_x FIRST:

Insert projector onto 'known' basis

$$r'_x = \langle \hat{x}' | r \rangle$$

$$= \langle \hat{x}' | \hat{x} \rangle \langle \hat{x} | r \rangle + \langle \hat{x}' | \hat{y} \rangle \langle \hat{y} | r \rangle$$

$$= \hat{x}' \cdot \hat{x}\, r_x + \hat{x}' \cdot \hat{y}\, r_y$$

$$= \cos\theta\, r_x - \sin\theta\, r_y$$

- LIKEWISE: $r'_y = \langle \hat{y}' | r \rangle$

$$= \langle \hat{y}' | \hat{x} \rangle \langle \hat{x} | r \rangle + \langle \hat{y}' | \hat{y} \rangle \langle \hat{y} | r \rangle$$

$$= \hat{y}' \cdot \hat{x}\, r_x + \hat{y}' \cdot \hat{y}\, r_y$$

$$= \sin\theta\, r_x + \cos\theta\, r_y$$

$$\boxed{\begin{pmatrix} r'_x \\ r'_y \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} r_x \\ r_y \end{pmatrix}}$$

$\hookrightarrow R(\theta) = U$

Summary

- Basis sets can be continuous or discrete
  - The important equations are:

$$1 = \sum_j |j\rangle\langle j| \qquad 1 = \int dx\, |x\rangle\langle x|$$

$$\langle j | k \rangle = \delta_{jk} \qquad \langle x | x' \rangle = \delta(x - x')$$

- Change of basis is simple with Dirac notation:
  1. Write unknown quantity
  2. Insert projector onto known basis
  3. Evaluate the transformation matrix elements
  4. Perform the required summations

$$\begin{aligned} C_j &= \langle u_j | \psi \rangle \\ &= \sum_k \langle u_j | k \rangle \langle k | \psi \rangle \\ &= \sum_j \langle u_j | k \rangle c_k \end{aligned}$$