LECTURE 15:

EIGENVALUES AND EIGENVECTORS

Prof. N. Harnew

University of Oxford

MT 2012

Outline: 15. EIGENVALUES AND EIGENVECTORS

15.1 Eigenvalue equations

- A linear operator A transforms vector $|\mathbf{x}\rangle$ into another vector $A|\mathbf{x}\rangle$. The components of A and $|\mathbf{x}\rangle$ are defined with respect to some N-dimensional basis vectors.
- An eigenvalue equation is one that transforms as

$$A|\mathbf{x}\rangle = \lambda|\mathbf{x}\rangle$$

  where λ is just a number (can be complex)

  - A has transformed $|\mathbf{x}\rangle$ into a multiple of itself
  - Vector $|\mathbf{x}\rangle$ is the *eigenvector* of the operator A
    λ is the *eigenvalue*.
  - The operator A will have in general a *series* of eigenvectors $|\mathbf{x_j}\rangle$ and eigenvalues λ_j.
- Write in matrix form:

$$Ax = \lambda x$$

  where A is an $N \times N$ matrix.
- In QM, often deal with *normalized* eigenvectors:
  $x^\dagger x = \langle\mathbf{x}|\mathbf{x}\rangle = 1$ (where $x^\dagger = x^{*T} \rightarrow$ Hermitian conjugate)

Eigenvalue equations continued

- Eigenvalue equation:

$$Ax = \lambda x \;=\; \lambda I x \quad (I \text{ is the unit matrix})$$

  - $Ax - \lambda I x = 0$
  - $(A - \lambda I)x = 0$
  - A set of linear simultaneous equations of degree N.

- Homogeneous equations only have a non-trivial solution (x_i non-zero) if the determinant

$$|A - \lambda I| = 0$$

15.1.1 Eigenvalues of inverse matrix

- $Ax_i = \lambda_i x_i$
  [Subscript *i* signifies multiple eigenvectors/values can exist]
- Multiply from LHS by A^{-1}
  - $A^{-1}Ax_i = \lambda_i A^{-1} x_i$
  - $A^{-1}A = I$ and on rearranging:
  - $A^{-1}x_i = \frac{1}{\lambda_i} x_i$
- Hence the eigenvectors are the same, but the eigenvalues become $\frac{1}{\lambda_i}$.

15.2 Finding eigenvalues and eigenvectors: example

$$|A - \lambda I| = 0$$

- Find the eigenvalues and eigenvectors of the real symmetric matrix

$$\begin{pmatrix} 1 & 1 & 3 \\ 1 & 1 & -3 \\ 3 & -3 & -3 \end{pmatrix} \tag{1}$$

(This is a special kind of Hermitian matrix $\rightarrow$ $A = A^{*T}$).

- First the eigenvalues:
start from $|A - \lambda I| = 0$

$$\text{gives} \quad \begin{vmatrix} 1-\lambda & 1 & 3 \\ 1 & 1-\lambda & -3 \\ 3 & -3 & -3-\lambda \end{vmatrix} = 0 \tag{2}$$

- $(1-\lambda)[(1-\lambda)(-3-\lambda) - 9]$
$-[(-3-\lambda) + 9] + 3[-3 - 3(1-\lambda)] = 0$

The Characteristic Equation

Simplify:

$$\begin{aligned}
& (1-\lambda)[(1-\lambda)(-3-\lambda)-9] - [(-3-\lambda)+9] + 3[-3-3(1-\lambda)] \\
= \; & (1-\lambda)[(-3+2\lambda+\lambda^2-9] - [6-\lambda] + [-9-9+9\lambda] \\
= \; & (-12+2\lambda+\lambda^2) + (12\lambda-2\lambda^2-\lambda^3) + (-24+10\lambda) \\
= \; & -\lambda^3-\lambda^2+24\lambda-36
\end{aligned}$$

Hence $\lambda^3+\lambda^2-24\lambda+36=0$

- This is called the *characteristic equation*.
- The LHS of the equation is called the *characteristic polynomial*.
- The roots of the characteristic polynomial are the eigenvalues of A.

Finding the roots

- $\lambda^3 + \lambda^2 - 24\lambda + 36 = 0$
- Top tip: If the cubic equation has integer roots, minus the roots must multiply up to 36. Use trial and error to find the first root $\rightarrow$ try integers which are factors of 36 (e.g. $1, -1, 2, -2, -3, 3$ etc). Plugging in numbers into the equation, in this case $\lambda = 2$, "works".
- $(\lambda - 2)(\lambda^2 + 3\lambda - 18) = 0$

  $(\lambda - 2)(\lambda - 3)(\lambda + 6) = 0$
- Hence the eigenvalues of the equation are $2, 3$ and -6.

Calculate the eigenvectors

- Take the first eigenvalue $\lambda_1 = 2$. Eigenvalues must satisfy:

$$\begin{pmatrix} 1 & 1 & 3 \\ 1 & 1 & -3 \\ 3 & -3 & -3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 2 \times \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \tag{3}$$

- Hence

$$\begin{array}{ccccccc} x_1 & + & x_2 & + & 3x_3 & = & 2x_1 \\ x_1 & + & x_2 & - & 3x_3 & = & 2x_2 \\ 3x_1 & - & 3x_2 & - & 3x_3 & = & 2x_3 \end{array} \rightarrow \begin{array}{ccccccc} -x_1 & + & x_2 & + & 3x_3 & = & 0 \\ x_1 & - & x_2 & - & 3x_3 & = & 0 \\ 3x_1 & - & 3x_2 & - & 5x_3 & = & 0 \end{array} \tag{4}$$

- Only 2 independent equations:

$$\begin{array}{ccccccc} x_1 & - & x_2 & - & 3x_3 & = & 0 \\ 3x_1 & - & 3x_2 & - & 5x_3 & = & 0 \end{array} \tag{5}$$

- Immediately yields $x_3 = 0$ and $x_1 = x_2 \;\; (= k$ say$)$
- The eigenvector becomes

$$\begin{pmatrix} k \\ k \\ 0 \end{pmatrix} \tag{6}$$

Normalization

- Normalize $\rightarrow \quad k^2 + k^2 + 0 = 1 \quad \rightarrow k = \frac{1}{\sqrt{2}}$
- The normalized eigenvector is then $$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} \tag{7}$$
- Solve the other two eigenvector equations:

$$\begin{pmatrix} 1 & 1 & 3 \\ 1 & 1 & -3 \\ 3 & -3 & -3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 3 \times \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \tag{8}$$

$$\text{and} \quad \begin{pmatrix} 1 & 1 & 3 \\ 1 & 1 & -3 \\ 3 & -3 & -3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = -6 \times \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \tag{9}$$

- which gives the results for the other two eigenvectors (after normalization):

$$\begin{pmatrix} \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \end{pmatrix} \tag{10}$$

Vector orthogonality

- We will see later that the eigenvectors are orthogonal for a Hermitian matrix.
- Check this: $\langle \mathbf{x_i} | \mathbf{x_j} \rangle = \mathbf{x_i^*}^{\mathbf{T}} \mathbf{x_j}$ must equal 0

$$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0) \begin{pmatrix} \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0) \begin{pmatrix} \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \end{pmatrix} \quad (11)$$

$$= (\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}) \begin{pmatrix} \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \end{pmatrix} = 0 \quad (12)$$

- So the orthogonality is OK

15.3 Eigenvalues and eigenvectors of an Hermitian matrix

15.3.1 Prove the eigenvalues of Hermitian matrix are real

- Take an eigenvalue equation $\rightarrow |\mathbf{x}\rangle$ is an N-dimensional vector
  $A|\mathbf{x}\rangle = \lambda|\mathbf{x}\rangle \quad \rightarrow$ Equ (1)
- Take Hermitian conjugate of both sides
  $(A|\mathbf{x}\rangle)^\dagger = \langle\mathbf{x}|A^\dagger = \lambda^*\langle\mathbf{x}| \quad$ [recall $(XY)^\dagger = Y^\dagger X^\dagger$ & $\langle\mathbf{x}| = |\mathbf{x}\rangle^{*T}$]
- Multiply on the right by $|\mathbf{x}\rangle$
  $\langle\mathbf{x}|A^\dagger|\mathbf{x}\rangle = \lambda^*\langle\mathbf{x}|\mathbf{x}\rangle$
- But by definition of Hermitian matrix : $A^\dagger = A$
  $\langle\mathbf{x}|A|\mathbf{x}\rangle = \lambda^*\langle\mathbf{x}|\mathbf{x}\rangle \quad \rightarrow$ Equ (2)
- Multiply (1) on the left by $\langle\mathbf{x}|$
  $\langle\mathbf{x}|A|\mathbf{x}\rangle = \lambda\langle\mathbf{x}|\mathbf{x}\rangle \quad \rightarrow$ Equ (3)
- Subtract (3) from (2)
  $$(\lambda^* - \lambda)\langle\mathbf{x}|\mathbf{x}\rangle = 0$$
- Hence since $\langle\mathbf{x}|\mathbf{x}\rangle \neq 0, \quad \lambda^* = \lambda \quad \rightarrow \quad \lambda$ is real.

15.3.2 Prove the eigenvectors of Hermitian matrix are orthogonal

- Consider two eigenvalues & eigenvectors satisfying
  $A|\mathbf{x_i}\rangle = \lambda_i|\mathbf{x_i}\rangle \quad \rightarrow$ Equ (4)
  $A|\mathbf{x_j}\rangle = \lambda_j|\mathbf{x_j}\rangle \quad \rightarrow$ Equ (5)
- Take Hermitian conjugate of (4)
  $\langle\mathbf{x_i}|A^\dagger = \lambda_i^*\langle\mathbf{x_i}|$
- Multiply on the right by $|\mathbf{x_j}\rangle$
  $\langle\mathbf{x_i}|A^\dagger|\mathbf{x_j}\rangle = \lambda_i^*\langle\mathbf{x_i}|\mathbf{x_j}\rangle \quad \rightarrow$ Equ (6)
- Multiply Equ (5) on the left by $\langle\mathbf{x_i}|$
  $\langle\mathbf{x_i}|A|\mathbf{x_j}\rangle = \lambda_j\langle\mathbf{x_i}|\mathbf{x_j}\rangle \quad \rightarrow$ Equ (7)
- By definition $A^\dagger = A$, and λ_i, λ_j are real. Subtract (6) $-$ (7)

$$(\lambda_i - \lambda_j)\langle\mathbf{x_i}|\mathbf{x_j}\rangle = 0$$

- Hence since $(\lambda_i \neq \lambda_j)$ $\quad \langle\mathbf{x_i}|\mathbf{x_j}\rangle = 0$ and the eigenvectors are orthogonal.