Lecture 6: Time Propagation

Outline:
• Ordinary functions of operators
  – Powers
  – Functions of diagonal operators

• Solving Schrödinger's equation
  – Time-independent Hamiltonian
  – The Unitary time-evolution operator
  – Unitary operators and probability in QM
  – Iterative solution
  – Eigenvector expansion

Ordinary Functions of Operators

• Let us define an `ordinary function', $f(x)$, as a function that can be expressed as a power series in $x$, with scalar coefficients:

$$f(x) = \sum_{n} f_n x^n$$

• When given an operator, $A$, as an argument, we define the result to be:

$$f(A) := \sum_{n} f_n A^n$$

• Examples:

$$\sin(A) = A - \frac{A^3}{3!} + \frac{A^5}{5!} - \frac{A^7}{7!} + ...$$

$$e^A = I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + ....$$

$$= \sum_{n=0}^{\infty} \frac{A^n}{n!}$$

• THM: A function of an operator is defined by its power series
Powers of Operators

• An operator raised to the zero\(^{th}\) power:
  \[ A^0 := I \]

• Positive integer powers:
  \[ A^1 := A \]
  \[ A^2 := AA \]
  \[ A^3 := AAA \]
  etc...

• Operator inversion:
  – The operator \( A^{-1} \) is defined via:
    \[ A^{-1} A := I \]
    \[ (A^{-1})^{-1} := A \]

• Negative powers:
  \[ A^{-n} := (A^{-1})^n \]

• Fractional powers:
  \[ A^{1/2} A^{1/2} := A \]
  \[ \frac{e(A)}{A} = A^{-1} f(A) = f(A) A^{-1} \]
  etc...

Eigenvalues of functions of operator

\[ f(A)|a\rangle = f(a)|a\rangle \]

proof:
\[ f(A)|a\rangle = \sum_n f_n A^n |a\rangle \]
\[ = \sum_n f_n A^{-1} a |a\rangle \]
\[ = \sum_n f_n a A^{-n} |a\rangle \]
\[ = \sum_n f_n a^n |a\rangle \]

\[ f(A)|a\rangle = f(a)|a\rangle \]
Functions of Diagonal Operators

• Diagonal operators have the form:

\[
D = 
\begin{pmatrix}
  d_1 & 0 & 0 & \cdots & 0 \\
  0 & d_2 & 0 & \cdots & 0 \\
  0 & 0 & d_3 & \cdots & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & 0 & \cdots & d_M
\end{pmatrix}
\]

• They can be expressed in Dirac notation as:

\[
D = \sum_{n=1}^{M} d_n |n\rangle\langle n|
\]

• Every operator is diagonal in the basis of its own eigenvectors

• They have the property:
  - let C and D be diagonal matrices

\[
CD = \sum_{n=1}^{M} \sum_{m=1}^{M} c_n d_m |n\rangle\langle n| |m\rangle\langle m|
\]

  From which it follows that:

\[
f(D) = 
\begin{pmatrix}
  f(d_1) & 0 & 0 & \cdots & 0 \\
  0 & f(d_2) & 0 & \cdots & 0 \\
  0 & 0 & f(d_3) & \cdots & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & 0 & \cdots & f(d_M)
\end{pmatrix}
\]

Solving Schrödinger's Equation

• When the Hamiltonian is not explicitly time-dependent, Schrödinger's Equation is readily integrated:

\[
\frac{d}{dt} |\psi(t)\rangle = -\frac{i}{\hbar} H |\psi(t)\rangle
\]

\[
|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle
\]

  Proof:

\[
\frac{d}{dt} e^{-iHt/\hbar} |\psi(0)\rangle = \frac{d}{dt} \sum_{m=0}^{\infty} \left(-\frac{i}{\hbar} H\right)^m \frac{t^m}{m!} |\psi(0)\rangle
\]

\[
= \sum_{m=1}^{\infty} \left(-\frac{i}{\hbar} H\right)^m \frac{mt^{m-1}}{m!} |\psi(0)\rangle
\]

\[
= -\frac{i}{\hbar} H \sum_{m=0}^{\infty} \left(-\frac{i}{\hbar} H\right)^m \frac{t^m}{m!} |\psi(0)\rangle
\]

\[
= -\frac{i}{\hbar} H e^{-iHt/\hbar} |\psi(0)\rangle
\]

\[
= -\frac{i}{\hbar} H |\psi(t)\rangle
\]
The Unitary Time-Evolution Operator

- In general, the time-evolution operator is defined as:
  \[ |\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle \]
  - The operator \( U(t,t_0) \) must be Unitary (\( U^\dagger = U^{-1} \)) to preserve the norm of \( |\psi(t)\rangle \)

- For the case where \( H \) is not explicitly time-dependent, we see from the exact solution that:
  \[ U(t,t_0) = e^{-iH(t-t_0)/\hbar} \]
  - In the more general case where \( H = H(t) \), the above is not necessarily valid
    - In this case we must find an equation for \( U(t,t_0) \).
    - We start from Schrödinger's Equation:
      \[ \frac{d}{dt} |\psi(t)\rangle = -\frac{i}{\hbar} H |\psi(t)\rangle \]
    - Which we now write as:
      \[ \frac{d}{dt} U(t,t_0)|\psi(t_0)\rangle = -\frac{i}{\hbar} H U(t,t_0)|\psi(t_0)\rangle \]
    - Since this must be true for any initial state, \( |\psi(t_0)\rangle \), it follows that:
      \[ \frac{d}{dt} U(t,t_0) = -\frac{i}{\hbar} H U(t,t_0) \]

Unitary Operators and probability in QM

Recall \( p_n := \langle \psi_n | \psi_\ell \rangle \)

\[ \sum_n p_n = \sum_n \langle \psi_n | \psi_\ell \rangle = \langle \psi_\ell | \psi_\ell \rangle = 1 \]

so \( \langle \psi_\ell | \psi_\ell \rangle = 1 \) since \( \sum_n p_n = 1 \)

(normalization to unity = sum over probability = one)

Unitary Operators:

- definition: \( U^\dagger = U^{-1} \)
  \[ \Rightarrow U^\dagger U = U U^\dagger = I \]
  \[ U^\dagger = U^{-1} = I \]

Hermitian operators ‘generate’ unitary operators

let \( U = e^{-iGt} \), where \( G^\dagger = G \)
\[ U^\dagger = e^{iG^\dagger} = e^{-iG} \Rightarrow U^\dagger U = e^{iG} e^{-iG} = e^{i0} = I \]

\[ \Rightarrow \text{to get } \dot{U} = 0, G = 0 \]
Solving the Time-Evolution Operator Equation

• Since \( |\psi(t_0)\rangle = U(t_0, t_0)|\psi(t_0)\rangle \), it is clear that:
  \[
  U(t_0, t_0) = 1 \quad \text{initial and on } U(t, t_0)
  \]

• The equation of motion:
  \[
  \frac{d}{dt} U(t, t_0) = -\frac{i}{\hbar} H(t) U(t, t_0)
  \]

• Can be formally integrated:
  \[
  U(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} dt' H(t') U(t', t_0)
  \]

• Or re-expressed via the definition of the derivative as:
  \[
  \frac{U(t + dt, t_0) - U(t_0)}{dt} = -\frac{i}{\hbar} H(t) U(t, t_0)
  \]
  \[
  U(t + dt, t_0) = \left[ 1 - \frac{i}{\hbar} H(t) dt \right] U(t_0)
  \]

• With \( t_0 = t \), this gives infinitesimal time evolution operator:
  \[
  U(t + dt, t) = 1 - \frac{i}{\hbar} H(t) dt
  \]

• So that (for numerical purposes):
  \[
  \lim_{N \to \infty} U(t, t_0) = \lim_{N \to \infty} U(t_0 + dt, t_0) \cdots U(t_i + dt, t_i) U(t_0 + dt, t_0)
  \]
  \[
  = \lim_{N \to \infty} \left[ 1 - \frac{i}{\hbar} H(t_0) dt \right] \cdots \left[ 1 - \frac{i}{\hbar} H(t_i) dt \right] \left[ 1 - \frac{i}{\hbar} H(t_0) dt \right]
  \]
  \[
  = \left[ 1 - \frac{i}{\hbar} H(t_0) dt \right] \cdots \left[ 1 - \frac{i}{\hbar} H(t_N) dt \right]
  \]
  \[
  \text{where } t_m = t_0 + m dt \quad \text{and} \quad dt = (t - t_0)/N
  \]
Can this be simplified further?

• We have found the most general result is

\[ U(t, t_0) = \lim_{N \to \infty} U(t_N + dt, t_N) \cdots U(t_1 + dt, t_1) U(t_0 + dt, t_0) \]

\[ = \lim_{N \to \infty} \left[ 1 - \frac{i}{\hbar} H(t_N) dt \right] \cdots \left[ 1 - \frac{i}{\hbar} H(t_1) dt \right] \left[ 1 - \frac{i}{\hbar} H(t_0) dt \right] \]

• This can be re-written as:

\[ U(t, t_0) = \lim_{N \to \infty} e^{-\frac{i}{\hbar} H(t_N) dt} \cdots e^{-\frac{i}{\hbar} H(t_1) dt} e^{-\frac{i}{\hbar} H(t_0) dt} \]

• Note that:

\[ e^A e^B = e^{A+B} \]

– Only in the case \([A,B]=0\)

• Thus can we write:

\[ U(t, t_0) = e^{-\frac{i}{\hbar} \int_{t_0}^{t} H(t') dt'} \]

– ONLY if the Hamiltonian satisfies:

\[ [H(t), H(t')] = 0 \ \forall \ t, t' \]

Iterative solution:

• We have:

\[ \frac{d}{dt} U(t, t_0) = -\frac{i}{\hbar} H(t) U(t, t_0) \]

• Start with:

\[ U_0(t, t_0) = I \]

• The iterative form of the equation is:

\[ \frac{d}{dt} U_{n+1}(t, t_0) = -\frac{i}{\hbar} H(t) U_n(t, t_0) \quad U(t, t_0) = U_\infty(t, t_0) \]

• Which gives

– Note: the “I” is an integration constant fitted to the initial conditions

\[ U_1(t, t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} H(t_1) dt_1 \]

• The final solution is:

\[ U(t, t_0) = I + \left( \frac{i}{\hbar} \right) \int_{t_0}^{t} dt_1 H(t_1) \]

\[ + \left( \frac{i}{\hbar} \right) \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 H(t_2) H(t_1) \]

\[ + \left( \frac{i}{\hbar} \right) \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_3 H(t_3) H(t_2) H(t_1) \]

\[ + \ldots \]
Eigenvector expansion

- For the case where $H$ is not explicitly time-dependent, it is most common to use the eigenvector basis to express the evolution operator.

  - The eigenvectors of $H$ are defined by the eigenvalue equation:

    $$H |\omega_n\rangle = \hbar \omega_n |\omega_n\rangle$$

  - Note the following:

    $$\sum_n |\omega_n\rangle \langle \omega_n | = 1$$

    $$\langle \omega_m | \omega_n \rangle = \delta_{mn}$$

    $$e^{-iHt/\hbar} |\omega_n\rangle = e^{-i\omega_n t} |\omega_n\rangle$$

Eigenvector Expansion cont.

- Start from:

  $$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle$$

- Apply the bra $\langle \omega_n |$ to:

  $$i\hbar \frac{d}{dt} \langle \omega_n | \psi(t) \rangle = \langle \omega_n | H | \psi(t) \rangle$$

  $$= \hbar \omega_n \langle \omega_n | \psi(t) \rangle$$

- Integration then gives:

  $$\langle \omega_n | \psi(t) \rangle = e^{-i\omega_n t} \langle \omega_n | \psi(0) \rangle$$

- We can express the state vector as:

  $$|\psi(t)\rangle = \sum_n |\omega_n\rangle \langle \omega_n | \psi(t) \rangle$$

  $$= \sum_n |\omega_n\rangle e^{-i\omega_n t} \langle \omega_n | \psi(0) \rangle$$
Summary

• Two approaches to solving Schrödinger's Equation:
  – Time-Evolution Operator:
    • Case I: $H(t) = H(0) = H$:
      \[
      \left| \psi(t) \right\rangle = e^{-iHt/\hbar} \left| \psi(0) \right\rangle
      \]
    • Case II: $H(t) \neq H(0)$, but $[H(t), H(t')] = 0$:
      \[
      \left| \psi(t) \right\rangle = e^{\frac{-i}{\hbar} \int_0^t H(t') \, dt'} \left| \psi(t_0) \right\rangle
      \]
  • Case II: $H(t) \neq H(0)$, but $[H(t), H(t')] = 0$:
    \[
    \left| \psi(t) \right\rangle = \lim_{N \to \infty} U(t_N + dt, t_N) \ldots U(t_1 + dt, t_1) U(t_0 + dt, t_0) \left| \psi(0) \right\rangle
    \]
  – Eigenvalue expansion:
    \[
    \left| \psi(t) \right\rangle = \sum_n \left| \omega_n \right\rangle e^{-i\omega_n t} \langle \omega_n \left| \psi(0) \right\rangle
    \]