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:

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

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

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

- THM: *A function ~~s~~ of an operator is defined by its power series*

Powers of Operators

- An operator raised to the zeroth 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:

$$A^{-1}A := I$$
$$\left(A^{-1}\right)^{-1} := A$$

$\rightarrow AA^{-1} = I$

$\frac{B}{A}$ is bad in QM

- Negative powers:

$$A^{-n} := (A^{-1})^n$$

is $\frac{B}{A} = A^{-1}B$ or BA^{-1}

$\frac{f(A)}{A} = A^{-1}f(A) = f(A)A^{-1}$

- Fractional powers:

$$A^{1/2}A^{1/2} := A$$
$$etc...$$

Eigenvalues of functions of operators

let $A|a\rangle = a|a\rangle$

then $f(A)|a\rangle = f(a)|a\rangle$

proof:

$$f(A)|a\rangle = \sum_n f_n A^n |a\rangle$$
$$= \sum_n f_n A^{n-1} a |a\rangle$$
$$= \sum_n f_n a A^{n-1} |a\rangle$$
$$= \sum_n f_n a^2 A^{n-2} |a\rangle$$
$$\vdots$$
$$= \sum_n f_n a^n |a\rangle$$

$$\boxed{f(A)|a\rangle = f(a)|a\rangle}$$

Functions of Diagonal Operators

- Diagonal operators have the form:

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

Basis dependent property

- 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

$$C\,D=\sum_{n=1}^{M}\sum_{m=1}^{M} c_n d_m |n\rangle\langle n|m\rangle\langle m|$$

$$=\sum_{n=1}^{M} c_n d_n |n\rangle\langle n|$$

$c_n d_n \rightarrow$

$$\begin{pmatrix} c_1d_1 & 0 & 0 & \cdots \\ 0 & c_2d_2 & 0 & \cdots \\ 0 & 0 & \ddots & \\ \vdots & \vdots & & c_Md_M \end{pmatrix}$$

Diagonal

- 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:

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

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

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

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

$$=-\frac{i}{\hbar}He^{-iHt/\hbar}|\psi(0)\rangle$$

$$=-\frac{i}{\hbar}H|\psi(t)\rangle$$

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:

$$U(t,t_0) = e^{-iH(t-t_0)/\hbar}$$

note: add cI to H, $\Rightarrow$ global phase $e^{-ict/\hbar}$

Doesn't change physics → freedom to choose Energy zero

- 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:

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{h}H|\psi(t)\rangle$$

  - Which we now write as:

$$\frac{d}{dt}U(t,t_0)|\psi(t_0)\rangle = -\frac{i}{h}H\,U(t,t_0)|\psi(t_0)\rangle$$

  - Since this must be true for any initial state, $|\psi(t_0)\rangle$, it follows that:

$$\frac{d}{dt}U(t,t_0) = -\frac{i}{h}H\,U(t,t_0)$$

Unitary Operators and probability in QM

Recall $P_n := \langle\psi|n\rangle\langle n|\psi\rangle$

$$\sum_n P_n = \sum_n \langle\psi|n\rangle\langle n|\psi\rangle = \langle\psi|\psi\rangle$$

so $\langle\psi|\psi\rangle = 1$ since $\sum_n P_n = 1$ for probabilities

- normalization to unity $\Rightarrow$ sum over probabilities is one

Unitary Operators:

definition: $U^\dagger = U^{-1}$

$$\rightarrow \quad U^\dagger U = U^{-1}U = \mathbb{I}$$
$$UU^\dagger = UU^{-1} = I$$

Hermitian operators 'generate' unitary operators

let $U = e^{iG}$, where $G^\dagger = G$

$$U^\dagger = e^{-iG^\dagger} = e^{-iG} \rightarrow U^\dagger U = e^{iG}e^{-iG} = \mathbb{I}$$

$e^{i(G-G)}$ as $[G,G]=0$

why are Unitary Operators so important in QM?

A: let $|\psi'\rangle = U|\psi\rangle$ ← Unitary trans.

where $U^{\dagger} = U^{-1}$

then $\langle\psi'|\psi'\rangle = \langle\psi|U^{\dagger}U|\psi\rangle$

$= \langle\psi|\psi\rangle$

"Unitary Transformations" preserve the norm → conserve probability

Solving the Time-Evolution Operator Equation

- Since $|\psi(t_0)\rangle = U(t_0,t_0)|\psi(t_0)\rangle$, it is clear that:

$$U(t_0,t_0) = 1$$ ← initial cond. on $U(t,t_0)$

- The equation of motion:

$$\frac{d}{dt}U(t,t_0) = -\frac{i}{h}H(t)U(t,t_0)$$

- Can be formally integrated:

$$U(t,t_0) = 1 - \frac{i}{h}\int_{t_0}^{t} dt'\, H(t')U(t',t_0)$$

- Or re-expressed via the definition of the derivative as:

$$\frac{U(t+dt,t_0) - U(t,t_0)}{dt} = -\frac{i}{h}H(t)U(t,t_0)$$

$$U(t+dt,t_0) = \left[1 - \frac{i}{h}H(t)dt\right]U(t,t_0)$$

- With $t_0 = t$, this gives infinitesimal time evolution operator: $U(t+dt,t) = 1 - \frac{i}{h}H(t)dt$
- So that (for numerical purposes):

$$U(t,t_0) = \lim_{N\to\infty} U(t_N + dt, t_N)\ldots U(t_1+dt,t_1)U(t_0+dt,t_0)$$

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

  – Where $t_m = t_0 + m\,dt$ and $dt = (t - t_0)/N$

Can this be simplified further?

- We have found the most general result is

$$U(t,t_0) = \lim_{N\to\infty} U(t_N + dt, t_N)\ldots U(t_1 + dt, t_1)U(t_0 + dt, t_0)$$

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

- This can be re-written as:

$$U(t,t_0) = \lim_{N\to\infty} e^{-\frac{i}{\hbar}H(t_N)dt}\ldots e^{-\frac{i}{\hbar}H(t_2)dt}e^{-\frac{i}{\hbar}H(t_1)dt}$$

- Note that:

$$e^A e^B = e^{A+B}$$

  - Only in the case [*A*,*B*]=*0*

- Thus can we write:

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

  - ONLY if the Hamiltonian satisfies:

$$\left[H(t), H(t')\right] = 0 \;\forall\; t, t'$$

Iterative solution:

- We have:

$$\frac{d}{dt}U(t,t_0) = -\frac{i}{h}H(t)U(t,t_0)$$

- Start with:

$$U_0(t,t_0) = I$$

- The iterative form of the equation is:

$$\frac{d}{dt}U_{n+1}(t,t_0) = -\frac{i}{h}H(t)U_n(t,t_0) \qquad U(t,t_0) = U_\infty(t,t_0)$$

- Which gives
  - Note: the "*I*" is an integration constant fitted to the initial conditions

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

- The final solution is:

$$U(t,t_0) = I + \left(\tfrac{-i}{\hbar}\right)\int_{t_0}^{t} dt_1\, H(t_1)$$
$$+ \left(\tfrac{-i}{\hbar}\right)^2\int_{t_0}^{t} dt_2\int_{t_0}^{t_2} dt_1 H(t_2)H(t_1)$$
$$+ \left(\tfrac{-i}{\hbar}\right)^3\int_{t_0}^{t} dt_3\int_{t_0}^{t_3} dt_2\int_{t_0}^{t_2} dt_1 H(t_3)H(t_2)H(t_1)$$
$$+\ldots$$

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 $\langle\omega_n|$ → :

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

- 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: $H(t)=H(0)=H$:

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

    - Case II: $H(t)\neq H(0)$, but $[H(t),H(t\_)]=0$:

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')}|\psi(t_0)\rangle$$

    - Case II: $H(t)\neq H(0)$, but $[H(t),H(t\_)]=0$:

$$|\psi(t)\rangle = \lim_{N\to\infty} U(t_N+dt,t_N)\ldots U(t_1+dt,t_1)U(t_0+dt,t_0)|\psi(0)\rangle$$

  - Eigenvalue expansion:

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