Lecture # 15

Time evolution of the system's state

Let's say that at $t = t_0$ our system is in a state $|\alpha\rangle$. At what state is it going to be at some later time t? $\Rightarrow$ i.e. we need to find

$$|\alpha, t_0 ; t\rangle \; , \; t > t_0$$

$$\lim_{t \to t_0} |\alpha, t_0 ; t\rangle = |\alpha\rangle$$

Notation: $|\alpha, t_0 ; t_0\rangle \equiv |\alpha, t_0\rangle$

So, how does the transformation $|\alpha, t_0\rangle \Rightarrow |\alpha, t_0 ; t\rangle$ happen? $\Rightarrow$

$$|\alpha, t_0 ; t\rangle = \underbrace{\hat{U}(t, t_0)}_{\uparrow} |\alpha, t_0\rangle$$

time-evolution operator
or
propagator

unitary $\Leftarrow$

$\Downarrow$

$$\hat{U}^{+} \hat{U} = \hat{I}$$

$$\hat{U}(t_0, t_0) = \hat{I}$$

Recall from Lecture #11 that the generator of time translations is the Hamiltonian $\Rightarrow$

$$\hat{U}(t_0+dt, t_0) = \hat{I} - \frac{i}{\hbar}\hat{H}\,dt$$

Consider successive transformations: first from t_0 to t, described by $\hat{U}(t, t_0)$, and then from t to $t+dt$, described by $\hat{U}(t+dt, t)$ $\Rightarrow$

$$\underbrace{\hat{U}(t+dt, t)}_{\Downarrow}\,\hat{U}(t,t_0) = \hat{U}(t+dt, t_0)$$

$$= \left(\hat{I} - \frac{i}{\hbar}\hat{H}dt\right)\hat{U}(t,t_0) = \hat{U}(t,t_0) - \frac{i}{\hbar}dt\,\hat{H}\hat{U}(t,t_0)$$

$\Downarrow$

$$\underbrace{\hat{U}(t+dt, t_0) - \hat{U}(t,t_0)}_{\displaystyle = \frac{\partial}{\partial t}\hat{U}(t,t_0)\cdot dt} = -\frac{i}{\hbar}dt\,\hat{H}\hat{U}(t,t_0) \quad \Rightarrow$$

$$\underbrace{i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}\hat{U}(t,t_0)}_{} \qquad (15.1)$$

the Schroedinger equation for the propagator multiply by $|\alpha, t_0\rangle \Rightarrow$

$$i\hbar \frac{\partial}{\partial t} \underbrace{\hat{U}(t,t_0)|\alpha,t_0\rangle}_{\substack{\parallel \\ |\alpha,t_0;t\rangle}} = \hat{H} \underbrace{\hat{U}(t,t_0)|\alpha,t_0\rangle}_{\substack{\parallel \\ |\alpha,t_0;t\rangle}}$$

$$\Downarrow$$

$$i\hbar \frac{\partial}{\partial t}|\alpha,t_0;t\rangle = \hat{H}|\alpha,t_0;t\rangle \Rightarrow$$

Schroedinger equation!

Go back to $\hat{U}(t,t_0) \Rightarrow$

Can we integrate Eq. (15.1) out and find $\hat{U}(t,t_0)$? $\Rightarrow$ sure!

Case 1 $\quad \hat{H} \neq \hat{H}(t)$ (as in most "textbook" problems)

Then $\Rightarrow$ $\underline{\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}}$ (15.2)

Case 2 $\quad \hat{H} = \hat{H}(t)$, but $[\hat{H}(t_1), \hat{H}(t_2)] = 0$ for any t_1, t_2

$$\Downarrow$$

$$\underline{\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')}} \qquad (15.3)$$

this obviously turns into (15.2) if $\hat{H} \neq \hat{H}(t')$

Case 3 $[\hat{H}(t_1), \hat{H}(t_2)] \neq 0$ for arbitrary t_1, t_2

$\Downarrow$

$$\hat{U}(t,t_0) = \hat{I} + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n \, \hat{H}(t_1) \cdot \hat{H}(t_2) \ldots \hat{H}(t_n)$$

(15.4)

Dyson series

$\Downarrow$

used in time-dependent perturbation theory (Phys 653)

Homework:

Start from Eq. (15.4), make the assumption of $[\hat{H}(t_1), \hat{H}(t_2)] = 0$ and arrive at Eq. (15.3)

How do we propagate an arbitrary state $|\alpha\rangle$ in time? $\Rightarrow$ Consider a basis $\{|\varphi_n\rangle\}$ of eigenvectors of an operator $\hat{A}$, so that $\hat{A}|\varphi_n\rangle = a_n|\varphi_n\rangle$

If $[\hat{A}, \hat{H}] = 0 \Rightarrow \hat{A}$ & $\hat{H}$ share the same basis $\Rightarrow$

Hamiltonian, consider $\hat{H} \neq \hat{H}(t)$

$\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$.

As we know from before, we can expand an arbitrary state vector $|\alpha\rangle$ in terms of the base vectors $|\varphi_n\rangle$ as follows:

$$|\alpha\rangle = \sum_n \underset{\substack{\uparrow \\ t_0=0}}{c_n(0)}|\varphi_n\rangle$$

$\Rightarrow$ suppose this is the initial state at time $t_0 = 0$,

i.e. $|\alpha\rangle \equiv |\alpha, t_0=0\rangle$.

What is $|\alpha, t_0=0; t\rangle$? $\Longrightarrow$

$$|\alpha, t_0=0; t\rangle = \hat{U}(t, t_0=0)|\alpha, t_0=0\rangle =$$

$$= e^{-\frac{i}{\hbar}\hat{H}(t-\overset{=0}{t_0})}|\alpha, t_0=0\rangle =$$

$$= e^{-\frac{i}{\hbar}\hat{H}t}\sum_n c_n(0)|\varphi_n\rangle = \sum_n c_n(0)\, e^{-\frac{i}{\hbar}\hat{H}t}|\varphi_n\rangle$$

$$= \sum_n c_n(0)\, e^{-\frac{i}{\hbar}E_n t}|\varphi_n\rangle = \sum_n \underbrace{c_n(t)}_{=\,c_n(0)\,e^{-\frac{i}{\hbar}E_n t}}|\varphi_n\rangle$$

recall: if $\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$

$f(\hat{H})|\varphi_n\rangle = f(E_n)|\varphi_n\rangle$

What if at $t_0 = 0$, we are in one of the eigenstates $|\varphi_K\rangle$? $\Rightarrow$ $|\alpha, t_0 = 0\rangle = |\varphi_K\rangle \Rightarrow$

$$|\alpha, t_0 = 0; t\rangle = C_K(t)|\varphi_K\rangle = \underbrace{C_K(0)}_{=1} \cdot e^{-\frac{i}{\hbar}E_K t}|\varphi_K\rangle$$

$$= e^{-\frac{i}{\hbar}E_K t}|\varphi_K\rangle$$

$\Downarrow$

we are still at the same physical state $|\varphi_K\rangle$, but acquired the phase modulation $e^{-\frac{i}{\hbar}E_K t}$

So, general procedure to find time-evolution of $|\alpha\rangle$:

1) Find $\hat{A}$ such that $[\hat{A}, \hat{H}] = 0$
2) Expand $|\alpha\rangle$ in terms of $\{|\varphi_n\rangle\}$
3) Change $C_n(0)$ to $C_n(0)e^{-\frac{i}{\hbar}E_n t}$

<u>Example</u>

Consider a system whose initial state $|\Psi(0)\rangle$ is $|\Psi(0)\rangle = |\alpha, t_0 = 0\rangle \doteq \frac{1}{5}\begin{bmatrix} 3 \\ 0 \\ 4 \end{bmatrix}$

Hamiltonian is represented by

$$\hat{H} \doteq \begin{bmatrix} 3 & 0 & 0 \\ 0 & 0 & 5 \\ 0 & 5 & 0 \end{bmatrix}$$

Find the state of the system at a later time $t \Rightarrow$

1) Find eigenvectors of $\hat{H}$ $\Rightarrow$

$$\det\begin{bmatrix} 3-\lambda & 0 & 0 \\ 0 & -\lambda & 5 \\ 0 & 5 & -\lambda \end{bmatrix} = 0 \Rightarrow \quad \begin{array}{l} a)\ \lambda_1 = 3 \\ b)\ \lambda_{2,3} = \pm 5 \end{array}$$

$$|\varphi_1\rangle = |\lambda = 3\rangle \Rightarrow \begin{bmatrix} 0 & 0 & 0 \\ 0 & -3 & 5 \\ 0 & 5 & -3 \end{bmatrix}\begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = 0$$

C_1 - arbitrary

$-3C_2 + 5C_3 = 0 \Rightarrow$

$C_2 = -\frac{5}{3}C_3$

$$|\varphi_1\rangle \doteq \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$|\varphi_2\rangle = |\lambda = 5\rangle \Rightarrow \begin{bmatrix} -2 & 0 & 0 \\ 0 & -5 & 5 \\ 0 & 5 & -5 \end{bmatrix}\begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = 0$$

$$|\varphi_2\rangle \doteq \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \Leftarrow C_1 = 0,\ C_2 = C_3$$

$$|\varphi_3\rangle = |\lambda = -5\rangle \Rightarrow \begin{bmatrix} 8 & 0 & 0 \\ 0 & 5 & 5 \\ 0 & 5 & 5 \end{bmatrix}\begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = 0 \Rightarrow$$

$$|\varphi_3\rangle \doteq \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix} \Leftarrow C_1 = 0,\ C_2 = -C_3$$

2) Now expand $|\Psi(0)\rangle$ in terms of
Coefficients of expansion: $|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle$:

$$\langle \varphi_1 | \Psi(0)\rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 3 \\ 0 \\ 4 \end{bmatrix} \cdot \frac{1}{5} = \frac{3}{5}$$

$$\langle \varphi_2 | \Psi(0)\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 0 \\ 4 \end{bmatrix} \cdot \frac{1}{5} = \frac{4}{5\sqrt{2}}$$

$$\langle \varphi_3 | \Psi(0)\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} 3 \\ 0 \\ 4 \end{bmatrix} \cdot \frac{1}{5} = -\frac{4}{5\sqrt{2}}$$

So, $|\Psi(0)\rangle = \frac{3}{5}|\varphi_1\rangle + \frac{4}{5\sqrt{2}}|\varphi_2\rangle - \frac{4}{5\sqrt{2}}|\varphi_3\rangle$

3) Now propagate $|\Psi(0)\rangle$ in time:

$$|\Psi(t)\rangle \equiv |\alpha, t_0 = 0; t\rangle = \frac{3}{5} e^{-\frac{i}{\hbar}\cdot 3t} |\varphi_1\rangle + \frac{4}{6\sqrt{2}} e^{-\frac{i}{\hbar}\cdot 5t} |\varphi_2\rangle - \frac{4}{5\sqrt{2}} e^{\frac{i}{\hbar}\cdot 5t} |\varphi_3\rangle \doteq$$

$$\doteq \frac{1}{5}\begin{bmatrix} 3e^{-\frac{i}{\hbar}\cdot 3t} \\ \frac{4}{\sqrt{2}} e^{-\frac{i}{\hbar}\cdot 5t} \\ -\frac{4}{\sqrt{2}} e^{\frac{i}{\hbar}\cdot 5t} \end{bmatrix}$$