L20 - Unitaries from Time Evolution

5.10 Dynamics described by Unitary operators

5.10.1 Motivation

So far we look in dynamics to be able to determine a state at a later time t from its initial value following a very simple recipe:

Solution of Schrödinger's equation via Energy Eigenstates:

Step 1: find eigenvectors $|E_n\rangle$ and eigenvalue E_n of H

Step 2: Expand initial state in eigenbasis

$$|\Psi(0)\rangle = \sum_n c_n \, |E_n\rangle$$

Step 3: Write down solution

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

On the other hand, in Lecture 16 when we introduced the time evolution of states we started with some unitary operator describing how to initial and final state are connected:

$$|\Psi(t)\rangle = \mathcal{U}_t \, |\Psi(0)\rangle$$

which is convenient in order to find out the effect of the same time evolution for many different input states.

5.10.2 Unitary operator

We can find this unitary operator by writing the connection between input and output state in the coordinate representation with respect to the eigenbasis of the Hamiltonian:

$$\begin{pmatrix} c_1(t) \\ \vdots \\ c_n(t) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{E_1 t}{\hbar}} & & 0 \\ 0 & e^{-i\frac{E_2 t}{\hbar}} & \\ \vdots & & \ddots \\ 0 & 0 & e^{-i\frac{E_n t}{\hbar}} \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}$$

$$|\Psi(t)\rangle = \mathcal{U} \qquad |\Psi(0)\rangle$$

From this, we can read off the formal description of U:

$$\mathcal{U} = \sum_{k=1}^{n} e^{-i\frac{E_k t}{\hbar}} |E_k\rangle\langle E_k|$$

5.10.3 Unitary Operator as Exponential of Hamilton Operator

Let us compare the unitary operator to the Hamilton Operator H:

$$H = \sum_{k=1}^{n} E_k \, |E_k\rangle\langle E_k|$$

Let us now introduce an mathematical tool to make the connection:

Exponentiation of Operators

The exponential function can be expanded in a Taylor series as

$$e^{\alpha x} = \sum_{\ell=0}^{\infty} \frac{1}{\ell!} (\alpha x)^{\ell}$$

We can now use this notation to define the exponent of an operator as

$$e^{\mathcal{M}} := \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \mathcal{M}^{\ell}$$

Using this notation, we can now verify that

$$\mathcal{U} = e^{-i\frac{Ht}{\hbar}}$$

Proof:

$$e^{-i\frac{Ht}{\hbar}} = \sum_{\ell=0}^{\infty} \left(-\frac{it}{\hbar}\right)^{\ell} H^{\ell}$$

Multiplication of diagonal matrices!

$$= \sum_{\ell=0}^{\infty} \left(-\frac{it}{\hbar}\right)^{\ell} \sum_{k=0}^{n} E_k^{\ell} \, |E_k\rangle\langle E_k|$$

$$= \sum_{k=0}^{n} \left(\sum_{l=0}^{\infty} \left(-\frac{it}{\hbar}\right)^{l} E_k^{l} \right) |E_k\rangle\langle E_k|$$

$$= \sum_{k=0}^{n} e^{-i\frac{E_k t}{\hbar}} |E_k\rangle\langle E_k| = \mathcal{U}$$

5.10.4 Example:

Given an Hamilton Operator

$$H = \omega S_y$$

we find

Eigenvalues	$+\frac{\hbar\omega}{2}$	$-\frac{\hbar\omega}{2}$
Eigenvectors	$\|+\rangle_y$	$\|-\rangle_y$

5.10.4.1 Direct approach

Thus we have

$$\mathcal{U}_t = e^{-i\frac{\omega}{2}t} |+\rangle_{y\,y}\langle +| + e^{i\frac{\omega}{2}t} |-\rangle_{y\,y}\langle -|$$

We can translate this now into a coordinate representation. I choose the representation with respect to the z-basis, $\{|+\rangle, |-\rangle\}$

$$\mathcal{U}_t \doteq e^{-i\frac{\omega}{2}t} \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix} \frac{1}{\sqrt{2}}(1, -i)$$

$$+ e^{i\frac{\omega}{2}t} \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix} \frac{1}{\sqrt{2}}(1, i)$$

$$= e^{-i\frac{\omega}{2}t}\frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} + e^{i\frac{\omega}{2}t}\frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2}\left(e^{-i\frac{\omega}{2}t} + e^{i\frac{\omega}{2}t}\right) & \frac{1}{2}i\left(-e^{-i\frac{\omega}{2}t} + e^{i\frac{\omega}{2}t}\right) \\ \frac{1}{2}(-i)\left(-e^{-i\frac{\omega}{2}t} + e^{i\frac{\omega}{2}t}\right) & \frac{1}{2}\left(e^{-i\frac{\omega}{2}t} + e^{i\frac{\omega}{2}t}\right) \end{pmatrix}$$

$$= \begin{pmatrix} \cos\frac{\omega}{2}t & -\sin\frac{\omega}{2}t \\ \sin\frac{\omega}{2}t & \cos\omega t \end{pmatrix}$$

using
Euler's formula

$$e^{i\phi} = \cos\phi + i\sin\phi$$

$$\Rightarrow \cos\phi = \frac{1}{2}\left(e^{i\phi} + e^{-i\phi}\right)$$

$$\sin\phi = \frac{1}{2i}\left(e^{i\phi} - e^{-i\phi}\right)$$

5.10.4.2 Alternative approach:

From the definition of the Taylor series expansion of the operator exponentiation, it is easy to find the following formula which holds for all operators M such that

$$M^2 = \mathbb{1}$$

$$e^{iM\alpha} = \cos(\alpha)\,\mathbb{1} + i\sin(\alpha)\,M$$

In the above example we find

$$H = \omega S_y = \frac{\hbar}{2}\omega\,\sigma_y$$

where the Pauli Operator σ_y satisfies:

$$\sigma_y^2 = \mathbb{1}$$

so we have

$$U_t = e^{-i\frac{\omega t}{2}\sigma_y} = \cos\left(-\frac{\omega t}{2}\right)\mathbb{1} + i\sin\left(-\frac{\omega t}{2}\right)\sigma_y$$

$$= \cos\left(\frac{\omega t}{2}\right)\mathbb{1} - i\sin\left(\frac{\omega t}{2}\right)\sigma_y$$

Inserting the coordinate representation of the operators and with respect to the standard basis, we find

$$U_t \doteq \begin{pmatrix} \cos\frac{\omega t}{2} & -\sin\left(\frac{\omega t}{2}\right) \\ \sin\frac{\omega t}{2} & \cos\frac{\omega t}{2} \end{pmatrix}$$