Quantum Dynamics:

Now we are going to discuss how a quantum state evolves in time. In otherwords we are now concerned with the quantum mechanical analouge of Newton's equation (or Lagrange's or Hamilton's) ~~equation~~ of motion.

Time evolution and Schrödinger equation:

The first important point we should keep in mind, that time is just a parameter in quantum mechanics, not an operator.

The time evolution operator:

Our basic concern in this section is, how does a state ket change in time.

Let us consider a quatum state evolving in time from t_0 to t as

$$|\alpha, t_0; t\rangle \quad \text{for } (t > t_0).$$

Because time is assumed to be a continuous parameter, we have.

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

Let us consider the time evolution operator to be $U(t, t_0)$. Therefore

$$|\alpha, t_0; t\rangle = U(t, t_0)|\alpha, t_0\rangle$$

The first requirement is that of probability conservation.

Let us consider $|\alpha, t_0\rangle = \sum_{a'} c_{a'}(t_0) |a'\rangle$.

Similarly we have $|\alpha, t_0; t\rangle = \sum_{a'} c_{a'}(t) |a'\rangle$.

In general $|c_{a'}(t_0)| \neq |c_{a'}(t)|$.

But for conservation of probability requires $\sum_{a'} |c_{a'}(t)|^2 = \sum_{a'} |c_{a'}(t_0)|^2 = 1$.

which is followed by:

$$\langle \alpha, t_0; t | \alpha, t_0; t\rangle = \langle \alpha, t_0 | \alpha, t_0\rangle.$$

$$\Rightarrow \quad \langle \alpha, t_0 | U^\dagger(t, t_0)\, U(t, t_0) | \alpha, t_0\rangle = \langle \alpha, t_0 | \alpha, t_0\rangle$$

$$\Rightarrow \quad U^\dagger(t, t_0)\, U(t, t_0) = \mathbb{1}.$$

i.e. $U(t, t_0)$ is a unitary operator.

It is one of the most fundamental property of $U(t, t_0)$.

(Later in this course we will learn that there is a more general operation in quantum processes, which includes dissipation and other losses :).

The second important property is that of composition:

$$U(t_2, t_0) = U(t_2, t_1)\, U(t_1, t_0) \quad (t_2 > t_1 > t_0)$$

This equation says that if we are interested in obtaining time evolution from t_0 to t_2, then we can obtain the same result by dividing it from t_0 to t_1 and then t_1 to t_2, where t_1 is any arbitrary intermediate time. This process can be repeated arbitrary number of times.

In a more general quantum process, this property is referred to as divisibility property.

It turns out ~~that~~ to be advantageous to consider an infinitisimal time evolution $U(t_0 + dt, t_0)$:

$$|\alpha, t_0; t_0 + dt\rangle = U(t_0 + dt, t_0)\, |\alpha, t\rangle$$

where

$$\lim_{dt \to 0} U(t_0 + dt, t_0) = \mathbb{I}.$$

These requirements are satisfied by

$$U(t_0 + dt, t_0) = \mathbb{I} - i\Omega\, dt,$$

where Ω is a hermitian operator, and $dt \to 0$, such that higher order of dt can be safely ignored.

Unitarity :

$$U^{\dagger}(t_0 + dt, t_0)\, U(t_0 + dt, t_0)$$

$$= (\mathbb{I} + i\Omega\, dt)(\mathbb{I} - i\Omega\, dt)$$

$$= \mathbb{I} + i\Omega\, \cancel{dt} - i\Omega\, \cancel{dt} + \cancel{\Omega^2\, dt^2} \quad \text{ignore}$$

$$= \mathbb{I}.$$

Composition :

$$U(t_0 + dt_1 + dt_2, t_0) = U(t_0 + dt_1 + dt_2, t_0 + dt_1) \cdot U(t_0 + dt_1, t_0).$$

Proof :

$$U(t_0 + dt_1 + dt_2, t_0) = \mathbb{I} - i\Omega(t_0 + dt_1 + dt_2 - t_0).$$

$$= \mathbb{I} - i\Omega(t_0 + dt_1 + dt_2 - dt_1 - t_0)$$
$$- i\Omega(dt_1 + t_0 - t_0).$$

$$= U(t_0 + dt_1 + dt_2, t_0 + dt_1)$$
$$U(t_0 + dt_1, t_0).$$

(Proved).

To sum up, the infinitisimal time evolution operator can be written as

$$U(t_0 + dt, t_0) = \mathbb{I} - \frac{iH\,dt}{\hbar}$$

where the hermitian operator H is called the Hamiltonian.

The Schrödinger equation:

We are now in a position to derive the fundamental differential equation for the time evolution operator $U(t, t_0)$.
Using the composition property we have

$$U(t+dt, t_0) = U(t+dt, t)\, U(t, t_0)$$
$$= \left(\mathbb{I} - \frac{iH\,dt}{\hbar}\right) U(t, t_0).$$

$$\Rightarrow \quad U(t+dt, t_0) - U(t, t_0) = -\frac{iH\,dt}{\hbar}\, U(t, t_0).$$

$$\Rightarrow \quad \lim_{dt \to 0} \frac{U(t+dt, t_0) - U(t, t_0)}{dt} = -\frac{iH}{\hbar}\, U(t, t_0).$$

$$\Rightarrow \quad i\hbar \frac{\partial}{\partial t} U(t, t_0) = H\, U(t, t_0)$$

Multiplying $|\alpha, t_0\rangle$ on the right side:

$$i\hbar \frac{\partial}{\partial t} U(t, t_0)\, |\alpha, t_0\rangle = H\, U(t, t_0)\, |\alpha, t_0\rangle$$

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

Energy eigenkets:

To be able to evaluate the effect of the time evolution operator on a general initial ket $|\alpha\rangle$, we must know how it acts on the base kets used in expanding $|\alpha\rangle$.

This is particularly straightforward if the base kets used are eigenkets of A such that

$$[A, H] = 0.$$

then the eigenkets of A are also the eigenkets of H, called "energy eigenkets", whose eigenvalues are $E_{a'}$:

$$H|a'\rangle = E_{a'}|a'\rangle$$

We can now expand $\exp\left(-\frac{iHt}{\hbar}\right)$ in terms of $|a'\rangle\langle a'|$.

$$\exp\left(-\frac{iHt}{\hbar}\right) = \exp\left[-\frac{it}{\hbar}\sum E_{a'}|a'\rangle\langle a'|\right].$$

$$= \mathbb{I} - \frac{i}{\hbar}\sum_{a'} E_{a'}|a'\rangle\langle a'| + \left(-\frac{i}{\hbar}\right)^2 \sum_{a'} E_{a'}^2 |a'\rangle\langle a'| + \cdots$$

$$= \sum_{a'} |a'\rangle\langle a'| - \frac{i}{\hbar}\sum_{a'} E_{a'}|a'\rangle\langle a'| + \left(-\frac{i}{\hbar}\right)^2 \sum_{a'} E_{a'}^2|a'\rangle\langle a'| + \cdots$$

$$= \sum_{a'} \exp\left(-\frac{iE_{a'}t}{\hbar}\right)|a'\rangle\langle a'|.$$

Therefore

$$|\alpha, t_0=0; t\rangle = \exp\left(\frac{-iHt}{\hbar}\right)|\alpha\rangle$$

$$= \exp\left(\frac{-iHt}{\hbar}\right)\sum_{a'} |a'\rangle\langle a'|\alpha\rangle$$

$$|\alpha, t\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \exp\left(\frac{-iE_{a'}t}{\hbar}\right).$$

In other words, the expansion coefficients.

$$\langle a'|\alpha, t\rangle = \langle a'|\alpha\rangle \exp\left(\frac{-iE_{a'}t}{\hbar}\right).$$

$$C_{a'}(t) = C_{a'}(0) \exp\left(\frac{-iE_{a'}t}{\hbar}\right).$$

Time <u>dependence</u> of expectation values:

Let us consider $|a, t\rangle = U(t,0)|a\rangle$.

Therefore $\langle B\rangle_{|\alpha,t\rangle} = \langle a,t|B|a,t\rangle$

$$= \langle a|U^\dagger(t,0)|B|U(t,0)|a\rangle.$$

$$= \langle a|e^{iE_a t/\hbar} B\, e^{-iE_a t/\hbar}|a\rangle.$$

$$= \langle a|B|a\rangle$$

So the expectation value of an observable taken with respect to an energy eigenket does not change in time.

Case I: Hamiltonean independent of time.

$$U(t, t_0) = \mathbb{I} - \frac{iH}{\hbar}(t-t_0) \; ; \text{ when } t-t_0 = \Delta t$$

to be very small.

When $t - t_0 = N\Delta t$, we have

$$U(t, t_0) = U(t, t_0 - \Delta t) \cdot U(t_0 - \Delta t, t_0 - 2\Delta t) \cdot \ldots \cdot U(t-(N-1)\Delta t, \cancel{(N-\Delta t)} \; t_0 - (N-1)\Delta t)$$

$$= \lim_{N \to \infty} \left[\mathbb{I} - (iH/\hbar)\frac{(t-t_0)}{N} \right]^N$$

$$U(t, t_0) = \exp\left(-\frac{iH(t-t_0)}{\hbar}\right).$$

It can be checked that the given function satisfies all the properties of unitary operators.

Case II: Hamiltonean dependent on time

$$U(t, t_0) = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \, H(t')\right].$$

The situation is more interesting, when the expectation value is taken with respect to a superposition of energy eigenkets.

$$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle .$$

$$\langle \hat{B} \rangle = \left[\sum_{a'} c_{a'}^{*} \langle a' | \exp\left(\frac{iE_{a'}t}{\hbar}\right) \right] \cdot \hat{B} \cdot \left[\sum_{a''} c_{a''} \exp\left(\frac{iE_{a''}t}{\hbar}\right) |a''\rangle \right] .$$

$$= \sum_{a', a''} c_{a'}^{*} c_{a''} \langle a' | \hat{B} | a'' \rangle \exp\left[\frac{-i(E_{a''} - E_{a'})t}{\hbar} \right]$$

So this time the expectation value consists of oscillating terms with angular frequency

$$\omega_{a''a'} = \frac{E_{a''} - E_{a'}}{\hbar} .$$

Spin precession:

It is appropriate to consider an example in this situation.

We start with a Hamiltonean of a spin 1/2 system with (magnetic) moment $e\hbar/2m_e c$ subjected to an external magnetic field $\hat{B}$.

$$\hat{H} = -\left(\frac{e}{m_e c}\right)\hat{S}\cdot\hat{B} \qquad (e < 0 \text{ for electron}).$$

where
$$\hat{S} = \hat{S}_x\hat{x} + \hat{S}_y\hat{y} + \hat{S}_z\hat{z}$$
$$\hat{B} = \hat{B}_x\hat{x} + \hat{B}_y\hat{y} + B_z\hat{z}.$$

Furthermore consider $\hat{B} = B_z\hat{z}$ and B_z is independent of time and uniform along z-direction.

$$\therefore \quad \hat{H} = -\left(\frac{eB}{m_e c}\right)\hat{S}_z \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

$$\hat{H} = \mp\frac{e\hbar B}{2m_e c}$$

It is convenient to define ω in such a way that the difference between two energy eigenvalues is $\hbar\omega$.

~~That~~ with $\omega = \dfrac{|e|B}{m_e c}$

Therefore $H = \omega S_z$

and $U(t,0) = \exp\left(-\frac{i\omega S_z t}{\hbar}\right)$

we apply this to the initial ket vector

$$|\alpha\rangle = c_+ |1\rangle + c_- |0\rangle$$

We have,

$$H|1\rangle = \frac{\hbar\omega}{2}|1\rangle$$

$$H|0\rangle = -\frac{\hbar\omega}{2}|0\rangle$$

Therefore

$$|\alpha, t\rangle = U(t,0)|\alpha\rangle$$

$$= c_+ \exp\left(-\frac{i\omega t}{2}\right)|1\rangle + c_- \exp\left(\frac{i\omega t}{2}\right)|0\rangle$$

Consider $c_+ = c_- = \frac{1}{\sqrt{2}}$.

The probabities of finding the state in

$$|S_x, \pm\rangle = \frac{|1\rangle \pm |0\rangle}{\sqrt{2}}$$

$$P_\pm = |\langle S_x, \pm | \alpha, t\rangle|^2$$

$$= \left| \left[\frac{\langle 1| \pm \langle 0|}{\sqrt{2}}\right]\left[\frac{1}{\sqrt{2}} e^{-i\omega t/\hbar}|1\rangle + \frac{1}{\sqrt{2}} e^{i\omega t/2}|0\rangle\right]\right|^2$$

$$= \left| \frac{e^{-\frac{i\omega t}{2}} \pm e^{\frac{i\omega t}{2}}}{2} \right|^2$$

$$= \begin{cases} \cos^2 \omega t/2, & \text{for } |S_x +\rangle \\ \sin^2 \omega t/2 & \text{for } |S_x -\rangle \end{cases}$$