Quantum dynamics

(11)

1. Schrödinger picture

The basic question of nonrelativistic ~~quant~~ quantum dynamics is: given an initial state $|\psi(t_0)\rangle$ of the system, how the state at time t, $|\psi(t)\rangle$, is determined. The assertion that $|\psi(t_0)\rangle$ determines $|\psi(t)\rangle$ is the quantum mechanical form of the principle of causality, and we shall assume it.

In addition, we postulate an extension of the principle of superposition to include the temporal development of states. This states that if $|\psi_1(t_0)\rangle$ and $|\psi_2(t_0)\rangle$ separately evolve into $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$, then a superposition

$$|\psi(t_0)\rangle = \lambda_1|\psi_1(t_0)\rangle + \lambda_2|\psi_2(t_0)\rangle$$

develops into

$$|\psi(t)\rangle = \lambda_1|\psi_1(t)\rangle + \lambda_2|\psi_2(t)\rangle,$$

i.e., each component of the state moves independently of each other. This means that $|\psi(t)\rangle$ can be obtained from an arbitrary initial state by the application of a linear operator:

$$|\psi(t)\rangle = T(t, t_0)\,|\psi(t_0)\rangle, \quad \cdots\cdots (1)$$

The operator T is called the time evolution operator for quantum mechanical state vectors.

Schrödinger equation.

The exact form of the time evolution operator can be found from the Schrödinger equation, which is a postulate of quantum mechanics describing how the state vector changes with time. The Schrödinger equation is

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H\,|\psi(t)\rangle \quad \cdots\cdots (2)$$

where H is a linear operator, called the Hamiltonian of the system.

Conservation of probability

First, we note that normalization of the state vector remains unchanged, i.e.,

$$\langle \psi(t) | \psi(t) \rangle = \langle \psi(t_0) | \psi(t_0) \rangle = 1 \quad \cdots \quad (3)$$

Proof: ~~Consider~~

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

$$= \left(i\hbar \frac{d}{dt} \langle \psi(t) | \right) | \psi(t) \rangle + \langle \psi(t) | \left(i\hbar \frac{d}{dt} | \psi(t) \rangle \right).$$

The Schrödinger equation in the dual space can be written as

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

since H is a hermitian operator. Hence we have

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

$$= - \langle \psi(t) | H | \psi(t) \rangle + \langle \psi(t) | H | \psi(t) \rangle$$

$$= 0$$

i.e.,

$$\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = 0$$

or $$\langle\psi(t)|\psi(t)\rangle = \text{contant} = \langle\psi(t_0)|\psi(t_0)\rangle.$$

QED.

To see that the constancy of the normalization of the state vector, implies conservation of probability, let us expand $|\psi(t_0)\rangle$ and $|\psi(t)\rangle$ as linear combinations of a complete basis set which we take to be the eigenkets of some observable A (in general a complete set of observables). Thus we write

$$|\psi(t_0)\rangle = \sum_{a'} c_{a'}(t_0)\,|a'\rangle \quad \text{------ (4)}$$

and

$$|\psi(t)\rangle = \sum_{a'} c_{a'}(t)\,|a'\rangle, \quad \text{---- (5)}.$$

Here $c_{a'}(t_0) \equiv \langle a'|\psi(t_0)\rangle$ is the probability amplitude that at time to a measurement of A will give the value a'. Similarly $c_{a'}(t) \equiv \langle a'|\psi(t)\rangle$

is the probability amplitude for obtaining a' at a later time t. In general, we do not expect the probability for obtaining a' to remain the same, i.e.,

$$|c_{a'}(t)|^2 \neq |c_{a'}(t_0)|^2.$$

However, the total probability must be 1 both at time t_0 and time t. Thus

$$\sum_{a'} |c_{a'}(t)|^2 = \sum_{a'} |c_{a'}(t_0)|^2 = 1 \quad \ldots\ldots (6)$$

since

$$\langle\psi(t)|\psi(t)\rangle = \sum_{a'} |c_{a'}(t)|^2$$

and

$$\langle\psi(t_0)|\psi(t_0)\rangle = \sum_{a'} |c_{a'}(t_0)|^2,$$

it follows that if the state ket is ~~normal~~ initially normalized to unity, it must remain normalized to unity at all later times.

This property is guaranteed if the time evolution operator $T(t, t_0)$ is unitary, since

$$\langle \psi(t) | \psi(t) \rangle = \langle \psi(t_0) | T^{\dagger}(t, t_0)\, T(t, t_0) | \psi(t_0) \rangle$$

$$= \langle \psi(t_0) | \psi(t_0) \rangle .$$

Thus we must have

$$T^{\dagger}(t, t_0) = T^{-1}(t, t_0) . \qquad \text{- - - - - (7)}$$

Time evolution operator.

As we have discussed previously, time evolution operator $T(t, t_0)$ is linear and unitary. Obviously, we must also have

$$T(t_0, t_0) = T(t, t) = \hat{\mathbb{1}} \qquad \text{------- (8)}$$

Composition property

Another feature we require of the operator T is the composition property. Since $T(t, t_0)$ does not depend on $|\psi(t_0)\rangle$, it follows that

$$|\psi(t_2)\rangle = T(t_2, t_1)|\psi(t_1)\rangle$$

$$= T(t_2, t_1)\, T(t_1, t_0)\, |\psi(t_0)\rangle$$

Since, moreover

$$|\psi(t_2)\rangle = T(t_2, t_0)\,|\psi(t_0)\rangle,$$

we immediately obtain

$$T(t_2, t_0) = T(t_2, t_1)\, T(t_1, t_0) \qquad \text{---- (9)}$$

$$(t_2 > t_1 > t_0)$$

This equation says that if we are interested in the time evolution from t_0 to t_2, then we can obtain the same result by first considering time evolution from t_0 to t_1 and then from t_1 to t_2.

Now, since $T(t_0, t_0) = 1$ and $T(t, t) = 1$, it follows from the composition law (Eq. (9)) that

$$T(t, t_0)\, T(t_0, t) = 1$$

$$T(t_0, t)\, T(t, t_0) = 1$$

Therefore,

$$\left[T(t, t_0)\right]^{-1} = T(t_0, t).$$

Furthermore, since $T(t, t_0)$ is unitary, we obtain

$$T^{+}(t, t_0) = T^{-1}(t, t_0) = T(t_0, t). \quad \text{----} (10)$$

Infinitesimal time-evolution operator.

It turns out to be advantageous to consider an infinitesimal time-evolution operator $T(t+dt,t)$ which is defined by

$$|\psi(t+dt)\rangle = T(t+dt,t)|\psi(t)\rangle \quad \text{-----}(11)$$

or

$$|\psi(t)\rangle + \frac{\partial|\psi(t)\rangle}{\partial t}dt = T(t+dt,t)|\psi(t)\rangle$$

Now, from the Schrödinger equation we have

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

Hence

$$\left(\hat{1} - \frac{i}{\hbar}H(t)dt\right)|\psi(t)\rangle = T(t+dt,t)|\psi(t)\rangle.$$

Therefore,

$$\boxed{T(t+dt,t) = \hat{1} - \frac{i}{\hbar}H(t)dt.} \quad \text{----}(12)$$

Differential equation for $T(t, t_0)$

The fundamental differential equation for the time evolution operator $T(t, t_0)$ can easily be inferred from the Schrödinger equation for state vectors:

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

or,

$$i\hbar \frac{\partial}{\partial t} T(t, t_0) |\psi(t_0)\rangle = H(t) T(t, t_0) |\psi(t_0)\rangle .$$

Since the above equation holds for any $|\psi(t_0)\rangle$, we can write

$$\boxed{i\hbar \frac{\partial}{\partial t} T(t, t_0) = H(t) T(t, t_0) .} \quad \cdots (13)$$

Alternatively, we can derive the differential equation ~~para~~ for the time-evolution operator using the composition property of the operator. Thus,

$$T(t+dt, t_0) = T(t+dt, t)\, T(t, t_0)$$

$$= \left(1 - \frac{i}{\hbar} H(t)\, dt\right) T(t, t_0)$$

or

$$\frac{T(t+dt, t_0) - T(t, t_0)}{dt} = -\frac{i}{\hbar} H(t)\, T(t, t_0).$$

In the limit $dt \to 0$, we have

$$\frac{\partial T(t, t_0)}{\partial t} = -\frac{i}{\hbar} H(t)\, T(t, t_0)$$

or

$$\boxed{i\hbar \frac{\partial T(t, t_0)}{\partial t} = H(t)\, T(t, t_0).}$$

This is the Schrödinger equation for the time-evolution operator.

Explicit form for the time-evolution operator.

We will now find an explicit formula for the time evolution operator. We will distinguish three cases:

1. H is independent of time
2. H depends on time but H at different times commute:

$$[H(t_1), H(t_2)] = 0$$

3. H depends on time and H at different times do not commute:

$$[H(t_1), H(t_2)] \neq 0.$$

Case 1 H independent of time.

Often H does not depend on time. Then it is easy to solve the Schrödinger equation for the time evolution operator:

$$i\hbar \frac{\partial}{\partial t} T(t, t_0) = H\, T(t, t_0)$$

with

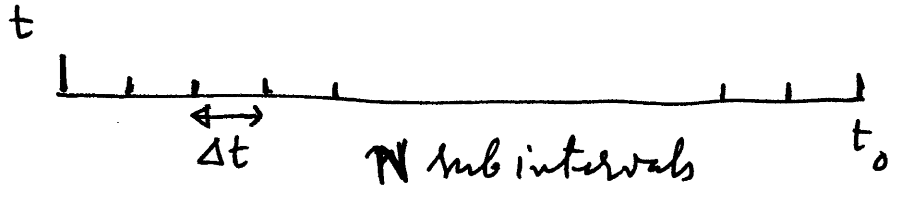
$$T(t_0, t_0) = \hat{\mathbb{1}}$$

If H is independent of time, then we can solve the above equation by inspection. We have

$$\boxed{\begin{array}{c} T(t, t_0) = e^{-\frac{i}{\hbar} H (t - t_0)} \\ \text{(H independent of time).} \end{array}} \qquad (13)$$

Another way to derive Eq. (13) is to successively compound infinitesimal time evolution operators as explained below:

We divide the full time interval $t - t_0$ into N equal ~~subinter~~ subintervals, each of duration $\Delta t = \frac{(t - t_0)}{N}$.



Since the Hamiltonian H is independent of time, the time evolution operator T in each subinterval Δt is the same, namely

$$T \approx \hat{1} - \frac{i}{\hbar} H \Delta t$$

The full time evolution operator from t_0 to t is then

$$T(t,t_0) \approx \underbrace{\left(1-\frac{i}{\hbar}H\Delta t\right)\left(1-\frac{i}{\hbar}H\Delta t\right)\cdots\cdot\left(1-\frac{i}{\hbar}H\Delta t\right)}_{N \text{ times}}$$

$$= \left[1-\frac{i}{\hbar}H\,\frac{(t-t_0)}{N}\right]^N$$

In the ~~[illegible]~~ limit $\Delta t \to 0$, i.e., $N \to \infty$, the above equation becomes an exact equality. Using the identity

$$\lim_{N\to\infty}\left(1+\frac{x}{N}\right)^N = e^x$$

we have

$$T(t,t_0) = \lim_{N\to\infty}\left[1-\frac{i}{\hbar}H\,\frac{(t-t_0)}{N}\right]^N$$

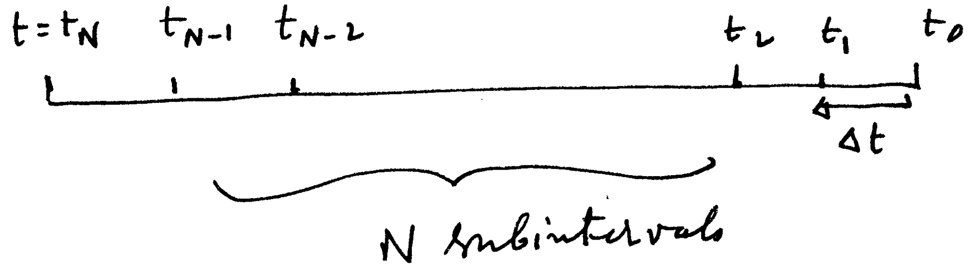
$$\boxed{T(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}}$$

Case 2

We now assume that H depends on time t. However, H at different instants commute

$$[H(t_1), H(t_2)] = 0 .$$

We proceed as before by dividing up the full time interval $t - t_0$ into N small subintervals each of duration $\Delta t = (t-t_0)/N$.



We label the final instant t as t_N and label the intermediate instants $t_1, t_2, \dots$ etc., as shown in the diagram above. Then we can write

$$T(t, t_0) = \underbrace{T(t_N, t_{N-1})\, T(t_{N-1}, t_{N-2}) \cdots T(t_2, t_1)\, T(t_1, t_0)}_{N \text{ terms}}$$

$$\approx \left(1 - \frac{i}{\hbar} H(t_{N-1}) \Delta t\right)\left(1 - \frac{i}{\hbar} H(t_{N-2}) \Delta t\right) \cdots$$

$$\cdots \left(1 - \frac{i}{\hbar} H(t_1) \Delta t\right)\left(1 - \frac{i}{\hbar} H(t_0) \Delta t\right)$$

Since Δt is small,

$$T(t,t_0) \simeq e^{-\frac{i}{\hbar}H(t_{N-1})\Delta t}\, e^{-\frac{i}{\hbar}H(t_{N-2})\Delta t} \cdots e^{-\frac{i}{\hbar}H(t_0)\Delta t}$$

Now we use the identity

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

if $[A,B]=0$. We get

$$T(t,t_0) \simeq e^{-\frac{i}{\hbar}\left(H(t_{N-1})\Delta t + H(t_{N-2})\Delta t + \cdots + H(t_1)\Delta t + H(t_0)\Delta t\right)}$$

The above equation becomes an equality in the limit $\Delta t \to 0$, i.e., $N \to \infty$. We then have

$$T(t,t_0) = \lim_{\Delta t \to 0} e^{-\frac{i}{\hbar}\sum_{i=0}^{N-1} H(t_i)\Delta t}$$

or

$$\boxed{T(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'}} \quad \cdots\cdots (14)$$

This is the time evolution operator if H is time dependent but H at different times commute. In the special case of time-independent Hamiltonian, Eq. (14) immediately leads to Eq. (13).

Case 3

Time dependent Hamiltonian and H at different instants do not commute.

In the case of non-commuting time-dependent Hamiltonian, we do not have a closed form for the time evolution operator. However, we can write down an infinite series for $T(t, t_0)$, each succeeding term of the series containing one extra H than the previous term. Such a series is called Dyson series.

We start with the differential equation satisfied by $T(t, t_0)$, (Eq. (13))

$$i\hbar \frac{\partial}{\partial t} T(t, t_0) = H(t)\, T(t, t_0) \quad \text{------ (15)}$$

with the initial condition

$$T(t_0, t_0) = \hat{\mathbb{1}} \quad \text{------ (16)}$$

It is convenient to convert the differential equation (15) into an integral equation in which we incorporate the initial condition (16).

The integral equation is

$$T(t,t_0) = \hat{1} - \frac{i}{\hbar}\int_{t_0}^{t} H(t')\,T(t',t_0)\,dt' \quad \text{-----(17)}$$

We can now iterate Eq. (17) to get an infinite series for $T(t,t_0)$. First, substitute $T(t',t_0)$, i.e., the left side of Eq (17) in the right hand side of Eq. (17). We get

$$T(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,H(t')\left(1 - \frac{i}{\hbar}\int_{t_0}^{t'} H(t'')\,T(t'',t_0)\,dt''\right)$$

~~This equation is still exact.~~

or

$$T(t,t_0) = \hat{1} - \frac{i}{\hbar}\int_{t_0}^{t} H(t')\,dt'$$

$$+\left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt'\,H(t')\int_{t_0}^{t'} H(t'')\,T(t'',t_0)\,dt'' \quad \text{---(18)}$$

This equation is still exact. Next, we again substitute $T(t'',t_0)$ from Eq. (17) into Eq. (18).

Continuing this process we get an infinite series for $T(t, t_0)$:

$$T(t,t_0) = \hat{\mathbb{1}} + \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t} H(t')\,dt'$$

$$+ \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, H(t')\,H(t'')$$

$$+ \left(-\frac{i}{\hbar}\right)^3 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \int_{t_0}^{t''} dt'''\, H(t')\,H(t'')\,H(t''')$$

$$+ \cdots$$

or

$$T(t,t_0) = \hat{\mathbb{1}} + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, H(t_1)H(t_2)\cdots H(t_n) \qquad \text{-----(19)}$$

We can write

$$T(t,t_0) = \sum_{n=0}^{\infty} T_n(t,t_0)$$

where

$$T_n(t,t_0) = \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \, H(t_1)\, H(t_2) \cdots H(t_n) .$$

Note that, in the above expression

$$t > t_1 > t_2 > t_3 \cdots t_1 > t_0$$

i.e., the operator $H(t_i)$ are placed in such a manner that H at an earlier time is on the right of H at ~~late~~ later times. We will now write $T_n(t,t_0)$ ~~in~~ such, that ~~a manner~~ that the limits of integration are the same for all integrals, the limits ~~be~~ being t_0 to t. For this we need the concept of time ordered product of operators.

Time ordered product of operators

The time-ordered product of two time-dependent operators is defined as

$$T\big(H(t_1)H(t_2)\big) = \begin{cases} H(t_1)\,H(t_2) & \text{if } t_1 > t_2 \\ H(t_2)\,H(t_1) & \text{if } t_2 > t_1 \end{cases} \qquad (20).$$

We now introduce the theta function $\theta(x)$ as

$$\theta(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 1 . \end{cases}$$

Therefore $\theta(t_1 - t_2)$ has the value 1 if $t_1 > t_2$ and the value 0 if $t_1 < t_2$. Using the theta function the time ordered product of two operators (Eq. (20)) can be written as

$$T\big(H(t_1)H(t_2)\big) = \theta(t_1 - t_2)H(t_1)H(t_2) + \theta(t_2 - t_1)H(t_2)H(t_1)$$

or

$$T\big(H(t_1)H(t_2)\big) = \sum_{\sigma \in S_2} \theta\left(t_{\sigma(1)} - t_{\sigma(2)}\right) H\left(t_{\sigma(1)}\right) H\left(t_{\sigma(2)}\right) \tag{21}$$

where σ's are elements of the permutation group of two objects 1 and 2. We have either

$$\sigma(1) = 1 \quad \& \quad \sigma(2) = 2$$

or

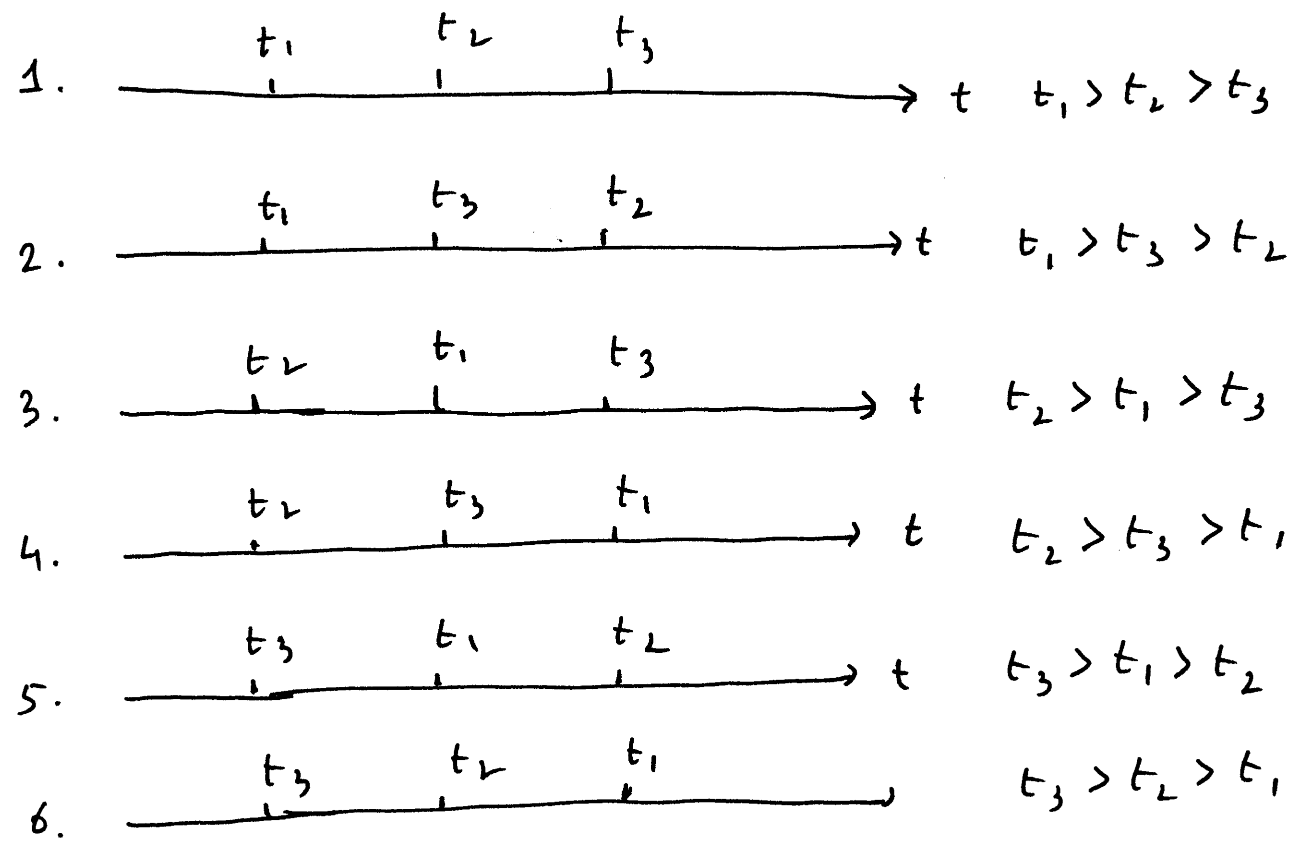
$$\sigma(1) = 2 \ \& \ \sigma(2) = 1$$

The first σ leaves the order of 1 & 2 unchanged (i.e., the identity operation) and the second σ interchanges 1 and 2 (a transposition). There are two elements of S_2 corresponding to the two σ's. In general, the permutation group of ~~three~~ n objects, S_n, has $n!$ elements.

Next, let us consider the time-ordered product of three operators

$$T\left(H(t_1) H(t_2) H(t_3) \right)$$

where each time argument t_i varies between t_0 and t. Now there are six possibilities for time ordering of t_1, t_2 and t_3 as shown in the diagram below.



There will be six terms in $T(H(t_1)H(t_2)H(t_3))$ corresponding to six different orderings of t_1, t_2, t_3. ~~All terms~~ The six orderings correspond to the action of the six elements of the permutation group S_3 on three objects t_1, t_2 and t_3. Thus, for example in the 4th ordering shown in the diagram above we have

$$\sigma(1) = 2, \quad \sigma(2) = 3, \quad \sigma(3) = 1$$

i.e., $\quad 1\,2\,3 \rightarrow 2\,3\,1$.

Written out in full, $T(H(t_1)H(t_2)H(t_3))$ is

$$\begin{aligned}
&T(H(t_1)H(t_2)H(t_3)) \\
&= \theta(t_1-t_2)\,\theta(t_2-t_3)\,H(t_1)H(t_2)H(t_3) \\
&+ \theta(t_1-t_3)\,\theta(t_3-t_2)\,H(t_1)H(t_3)H(t_2) \\
&+ \theta(t_2-t_1)\,\theta(t_1-t_3)\,H(t_2)H(t_1)H(t_3) \\
&+ \theta(t_2-t_3)\,\theta(t_3-t_1)\,H(t_2)H(t_3)H(t_1) \\
&+ \theta(t_3-t_1)\,\theta(t_1-t_2)\,H(t_3)H(t_1)H(t_2) \\
&+ \theta(t_3-t_2)\,\theta(t_2-t_1)\,H(t_3)H(t_2)H(t_1).
\end{aligned}$$

as

$$T\big(H(t_1)H(t_2)H(t_3)\big)$$

$$= \sum_{\sigma\in S_3} \theta(t_{\sigma(1)} - t_{\sigma(2)})\,\theta(t_{\sigma(2)} - t_{\sigma(3)})\,H(t_{\sigma(1)})H(t_{\sigma(2)})H(t_{\sigma(3)})$$

$$= \sum_{\sigma\in S_3} \prod_{i=1}^{2} \theta(t_{\sigma(i)} - t_{\sigma(i+1)}) \prod_{i=1}^{3} H(t_{\sigma(i)}) .$$

In a similar way, time-ordered product of n operators can be written as

$$T\big(H(t_1)H(t_2)\cdots H(t_n)\big)$$

$$= \sum_{\sigma\in S_n} \theta(t_{\sigma(1)} - t_{\sigma(2)})\,\theta(t_{\sigma(2)} - t_{\sigma(3)})\cdots\theta(t_{\sigma(n-1)} - t_{\sigma(n)})$$

$$\times H(t_{\sigma(1)})H(t_{\sigma(2)})\cdots H(t_{\sigma(n)}) .$$

$$= \sum_{\sigma\in S_n} \prod_{i=1}^{n-1} \theta(t_{\sigma(i)} - t_{\sigma(i+1)}) \prod_{i=1}^{n} H(t_{\sigma(i)})$$

We now return to the series solution of $T(t, t_0)$. ~~In Eq. (22) $t_2 < t_1$ < In Equations~~ (21) ~~and (22) we could change the limits of both~~ integrals ~~to t_0,~~

Time evolution operator again

Previously we derived the time evolution operator as

$$T(t, t_0) = \sum_{n=0}^{\infty} T_n(t, t_0)$$

where

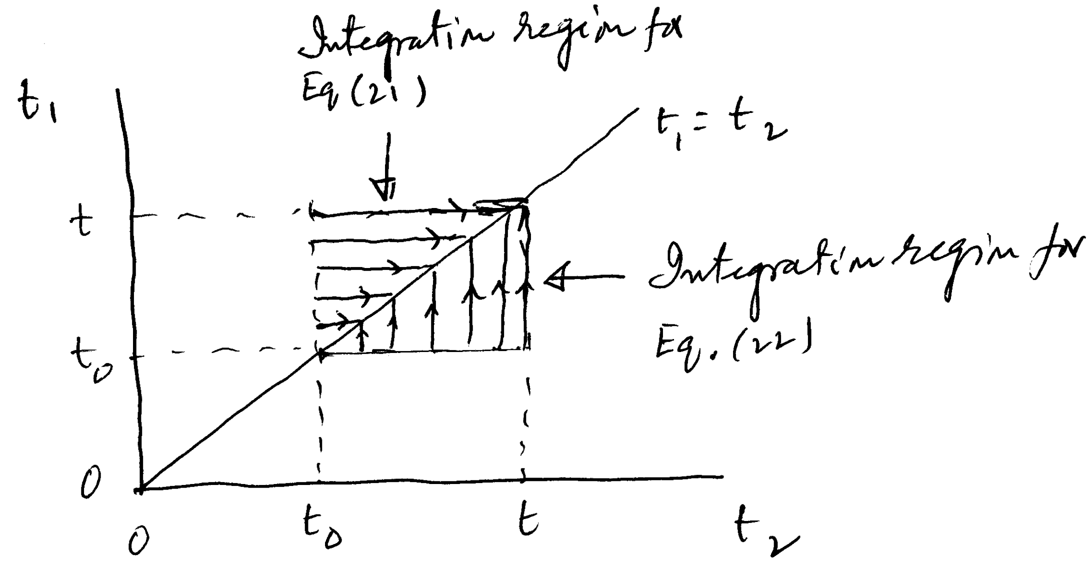
$$T_n(t, t_0) = \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \, H(t_1) H(t_2) \cdots H(t_n) \, .$$

To start our discussion let us consider the second order term $(n=2)$, i.e., the term containing $\hat{H}$ twice. This term is

$$T_2(t, t_0) = +\left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \, \hat{H}(t_1) \hat{H}(t_2) \quad \cdots\cdots (21)$$

Note that in this equations, the times t_1 and t_2 are ordered in such a way that ~~$H(t_1)$ is always on the~~ t_1 is always greater than or equal to t_2 and that $H(t_1)$ is on the left of $H(t_2)$. In other words H at a later time is always to the left of H at an earlier time. The region of integration in Eq. (21) is

Shown in figure below:



In the integral of Eq. (21) t_1 is varied from t_0 to t and for each t_1 in the range (t_0, t), t_2 is varied from t_0 to t_1 so that t_1 is always greater than or equal to t_2.

Now, in Eq. (21), t_1 and t_2 are dummy variables and the integral would remain unchanged if we interchange t_1 and t_2. Thus, we could write

$$\cancel{T_2 = \int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1\, H(t_2) H(t_1)} \quad \ldots$$

$$T_2 = \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1\, H(t_2) H(t_1) \quad \ldots \quad (22)$$

The integration region of Eq. (22) in the $t_1 - t_2$ plane is shown in the above figure.

Next, in Eqs. (21) and (22) we could make the integration limits symmetric ~~as~~ taking the limits in each integral from t_0 to t. Thus we can write Eqs. (21) and (22) as

$$T_2 = \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \ \theta(t_1 - t_2)\, H(t_1)\, H(t_2) \quad \cdots (23)$$

and

$$T_2 = \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_1 \ \theta(t_2 - t_1)\, H(t_2)\, H(t_1) \quad \cdots (24)$$

The theta functions are inserted because we have ensure that $t_1 > t_2$ in Eq. (23) and $t_2 > t_1$ in Eq. (24).

Since Eqs. (23) and (24) are identical, we have

$$T_2 = \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \Big[\theta(t_1 - t_2)\, H(t_1)\, H(t_2) + \theta(t_2 - t_1)\, H(t_2)\, H(t_1)\Big] \quad \cdots (25)$$

where we have used ~~that~~ the obvious fact that

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 = \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_1$$

if the limits for both dt_1 and dt_2 integrals are identical.

The integrand in Eq. (25) is the time ordered product $T(H(t_1)H(t_2))$. Thus, we can write Eq. (25) as

$$\boxed{T_2 = \frac{1}{2!}\left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \, T\left(H(t_1)H(t_2)\right)} \quad \cdots\cdots (26)$$

Third order term of $T(t, t_0)$

Now consider the third order term ($n = 3$) of the time evolution operator. This term is

$$T_3 = \left(-\frac{i}{\hbar}\right)^3 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 \; H(t_1)H(t_2)H(t_3), \quad \cdots (27)$$

The time ordering in the integral is $t_1 \geq t_2 \geq t_3$. We can write Eq. (27) as

$$T_3 = \left(-\frac{i}{\hbar}\right)^3 \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_3 \; \theta(t_1 - t_2)\,\theta(t_2 - t_3)\, H(t_1)H(t_2)H(t_3)$$

$$\cdots (28)$$

In Eq. (28) the limits of each integral is from t_0 to t, but the restriction $t_1 \geq t_2 \geq t_3$ is maintained by the theta functions.

As before, noting that t_1, t_2 and t_3 are dummy variables, we can permute them in any order ~~and~~ but T_3 will remain the same. In each permutation the integration region would remain the same because the limits for each variable are the same; but the integrand would change. Since there are 3! elements of the permutation group of three elements we could write

$$T_3 = (-i/\hbar)^3 \frac{1}{3!} \sum_{\sigma \in S_3} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_3$$

$$\times \; \Theta(t_{\sigma(1)} - t_{\sigma(2)})\, \Theta(t_{\sigma(2)} - t_{\sigma(3)})\, H(t_{\sigma(1)})\, H(t_{\sigma(2)})\, H(t_{\sigma(3)})$$

$$= (-i/\hbar)^3 \frac{1}{3!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_3$$

$$\times \sum_{\sigma \in S_3} \Theta(t_{\sigma(1)} - t_{\sigma(2)})\, \Theta(t_{\sigma(2)} - t_{\sigma(3)})\, H(t_{\sigma(1)})\, H(t_{\sigma(2)})\, H(t_{\sigma(3)})$$

$$\boxed{T_3 = \left(-i/\hbar\right)^3 \frac{1}{3!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_3 \; T\left(H(t_1) H(t_2) H(t_3) \right)} \qquad (27)$$

Next, let us consider the general n^{th} order term of the evolution operator.

$$T_n(t, t_0)$$
$$= \left(-i/\hbar\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \; H(t_1) H(t_2) \cdots H(t_n)$$

Since $t_1, t_2 \ldots t_n$ are dummy variables, we can permute them in any order without changing the value of T_n. Since there are $n!$ elements of the permutation group S_n of n objects, we have

$$T_n(t,t_0)$$

$$= \left(-i/\hbar\right)^n \frac{1}{n!} \sum_{\sigma \in S_n} \int_{t_0}^{t} dt_{\sigma(1)} \int_{t_0}^{t_{\sigma(1)}} dt_{\sigma(2)} \cdots \int_{t_0}^{t_{\sigma(n-1)}} dt_{\sigma(n)}\, H(t_{\sigma(1)}) \cdots H(t_{\sigma(n)})$$

$$= \left(-i/\hbar\right)^n \frac{1}{n!} \sum_{\sigma \in S_n} \int_{t_0}^{t} dt_{\sigma(1)} \int_{t_0}^{t} dt_{\sigma(2)} \cdots \int_{t_0}^{t} dt_{\sigma(n)}$$

$$\times\ \theta(t_{\sigma(1)} - t_{\sigma(2)})\, \theta(t_{\sigma(2)} - t_{\sigma(3)}) \cdots \theta(t_{\sigma(n-1)} - t_{\sigma(n)})$$

$$\times\ H(t_{\sigma(1)})\, H(t_{\sigma(2)}) \cdots H(t_{\sigma(n)})$$

$$= \left(-i/\hbar\right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n$$

$$\times \sum_{\sigma \in S_n} \Big[\theta(t_{\sigma(1)} - t_{\sigma(2)})\, \theta(t_{\sigma(2)} - t_{\sigma(3)}) \cdots \theta(t_{\sigma(n-1)} - t_{\sigma(n)})$$

$$\times\ H(t_{\sigma(1)})\, H(t_{\sigma(2)}) \cdots H(t_{\sigma(n)}) \Big]$$

$$= \left(-i/\hbar\right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n\; T\big(H(t_1)\, H(t_2) \cdots H(t_n)\big) \tag{28}$$

Hence, finally we have

$$T(t,t_0) = \sum_{n=0}^{\infty} T_n(t,t_0) \quad \text{---- (29)}$$

with $T_0(t,t_0) = \hat{\mathbb{1}}$ ---- (30)

and

$$T_n = (-i/\hbar)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n \, T(H(t_1)\cdots H(t_n))$$

$(n = 1, 2, \cdots)$, -- (31)

This is the Dyson perturbative formula for the time evolution operator. We can symbolically write this equation as

$$\boxed{T(t,t_0) = T e^{-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'}}^{\dagger} \quad (32)$$

† Note : There is a clash of notation here. The 'T' on the left means time evolution operator and T on the right means the time-ordered product.

Quantum dynamics contains no general prescription for the construction of the Hamiltonian operator $\hat{H}$ whose existence it asserts. The Hamiltonian operator must be found from experience, using the clues from classical description if one is available. Physical insight is required to make a judicious choice of operators in the description of the system (such as coordinates, momenta, spin variables, etc.) and to construct the Hamiltonian in terms of these variables

- Expectation values of observables in Schrödinger picture.

Contact with measurable quantities and classical concepts can be established if we calculate the time development of the expectation value of an operator A. We find

$$i\hbar \frac{d}{dt} \langle \psi(t) | \hat{A} | \psi(t) \rangle$$

$$= \left(i\hbar \frac{d}{dt} \langle \psi(t) | \right) \hat{A} \, | \psi(t) \rangle$$

$$+ \langle \psi(t) | \, i\hbar \frac{d\hat{A}}{dt} \, | \psi(t) \rangle$$

$$+ \langle \psi(t) | \hat{A} \left(i\hbar \frac{d}{dt} | \psi(t) \rangle \right)$$

Now, ~~from~~ the Schrödinger equation is

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

or, in the dual space

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

$\therefore \quad i\hbar \frac{d}{dt} \langle \psi(t) | \hat{A} | \psi(t) \rangle$

$$= - \langle \psi(t) | \hat{H} \hat{A} | \psi(t) \rangle$$

$$+ i\hbar \langle \psi(t) | \frac{\partial \hat{A}}{\partial t} | \psi(t) \rangle$$

$$+ \langle \psi(t) | \hat{A} \hat{H} | \psi(t) \rangle$$

$$= \langle \psi(t) | [\hat{A}, \hat{H}] | \psi(t) \rangle + i\hbar \langle \psi(t) | \frac{\partial \hat{A}}{\partial t} | \psi(t) \rangle$$

N $$\boxed{i\hbar \frac{d}{dt} \langle A \rangle (t) = \langle [A, H] \rangle + i\hbar \langle \frac{\partial \hat{A}}{\partial t} \rangle}$$

Normally, operators in the Schrödinger picture, ~~operators~~ are independent of time. Thus, if $\hat{A}$ is independent of time, then

$$\boxed{i\hbar \frac{d}{dt} \langle A \rangle = \langle [A, H] \rangle} \quad \ldots\ldots (33)$$

Thus, we see that commutators of $\hat{H}$ with observables play an important role in the theory. If A commutes with H, the expectation value of $\hat{A}$ is ~~to be a const~~ constant and A is said to be a constant of motion:

$$\boxed{\begin{array}{l} \text{If } \hat{A} \neq \hat{A}(t) \text{ and if} \\ \quad [\hat{A}, \hat{H}] = 0 \\ \text{Then } \quad \dfrac{d}{dt}\langle \hat{A} \rangle = 0 \\ \text{or } \langle \hat{A} \rangle = \text{constant} \\ \text{and the observable which corresponds to operator} \\ \hat{A} \text{ is constant of motion.} \end{array}}$$

Eq. (33) is called the Ehrenfest Theorem.

As an example we consider one-dimensional motion of a particle. Taking $\hat{A}$ in Eq.(33) to be $\hat{x}$, we have

$$\frac{d}{dt}\langle \hat{x} \rangle = -\frac{i}{\hbar} \langle [\hat{x}, \hat{H}] \rangle \quad \text{------} (34)$$

Now, $\hat{H}$ is of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

The commutator of $\hat{x}$ with $V(\hat{x})$ is zero, so we have to evaluate the commutator of $\hat{x}$ with $\frac{\hat{p}^2}{2m}$.

$$\left[\hat{x}, \frac{\hat{p}^2}{2m}\right] = \frac{1}{2m}[\hat{x}, \hat{p}^2]$$

$$= \frac{1}{2m}\left\{ \hat{p}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{p} \right\}$$

$$= \frac{1}{2m}\left\{ \hat{p}\, i\hbar + i\hbar\, \hat{p} \right\}$$

$$= \frac{i\hbar}{m}\hat{p}.$$

Hence

$$[\hat{x}, \hat{H}] = \frac{i\hbar}{m}\hat{p}.$$

Therefore, Eq. (34) becomes

$$\frac{d}{dt}\langle x\rangle = \left(-\frac{i}{\hbar}\right)\frac{i\hbar}{m}\langle \hat{p}\rangle$$

or

$$\boxed{\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}\rangle}{m}} \quad \text{--------- (35)}$$

In three dimensions we write

$$\frac{d\langle\hat{\vec{R}}\rangle}{dt} = \frac{\langle\hat{\vec{P}}\rangle}{m} \quad \text{------- (36)}$$

In classical mechanics we have

$$\frac{d\vec{r}}{dt} = \vec{v} = \frac{\vec{P}}{m}. \quad \text{------ (37)}$$

Next we consider $\frac{d}{dt}\langle \hat{p} \rangle$. From Eq. (33) we have

$$\frac{d\langle \hat{p} \rangle}{dt} = -\frac{i}{\hbar} \langle [\hat{p}, \hat{H}] \rangle \qquad (38)$$

We calculate

$$[\hat{p}, \hat{H}] = [\hat{p}, \frac{\hat{p}^2}{2m} + V(\hat{x})]$$

$$= [\hat{p}, V(\hat{x})]$$

To find $[\hat{p}, V(\hat{x})]$ we go to the coordinate basis in which

$$\hat{p} \rightarrow -i\hbar \frac{d}{dx} \qquad V(\hat{x}) \longrightarrow V(x)$$

and for any $\psi(x)$

$$[\hat{p}, V(\hat{x})]\psi(x)$$

$$= [-i\hbar \frac{d}{dx}, V(x)]\psi(x)$$

$$= -i\hbar \frac{d}{dx}\left(V(x)\psi(x)\right) + i\hbar V(x) \frac{d\psi(x)}{dx}$$

$$= -i\hbar \frac{dV(x)}{dx} \psi(x) .$$

Since $\psi(x)$ is arbitrary, we conclude that in the abstract

$$\left[\hat{P}, V(\hat{X})\right] = -i\hbar \frac{\partial V(\hat{X})}{\partial \hat{X}}$$

Therefore, Eq. (38) becomes

$$\frac{d}{dt}\langle \hat{P} \rangle = \left(-\frac{i}{\hbar}\right)\left(-i\hbar\right)\left\langle \frac{\partial V(\hat{X})}{\partial \hat{X}} \right\rangle$$

or $$\frac{d}{dt}\langle \hat{P} \rangle = -\left\langle \frac{dV(\hat{X})}{d\hat{X}} \right\rangle$$

or $$\frac{d\langle \hat{P} \rangle}{dt} = \left\langle -\frac{dV(\hat{X})}{d\hat{X}} \right\rangle \quad \cdots\cdots \quad (39)$$

In three dimensions we can write

$$\frac{d}{dt}\langle \hat{\vec{P}} \rangle = \langle -\vec{\nabla} V(\hat{\vec{R}}) \rangle . \quad \cdots\cdots \quad (40)$$

In Newtonian mechanics, Newton's second law

is $$\frac{d\vec{P}}{dt} = \vec{F} = -\vec{\nabla} V \quad \cdots\cdots \quad (41)$$

Thus in formulas of classical mechanics, if we replace the variables x and p by the expectation values of the corresponding operators, we get the quantum version of the classical equations. Note that, since $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, we could write Eqs. (35) and (39) as

$$\frac{d}{dt}\langle \hat{x} \rangle = \left\langle \frac{\partial \hat{H}}{\partial \hat{p}} \right\rangle \quad \text{......} \quad (42)$$

and

$$\frac{d}{dt}\langle \hat{p} \rangle = \left\langle -\frac{\partial \hat{H}}{\partial \hat{x}} \right\rangle, \quad \text{.....} \quad (43)$$

This two equations have striking similarity with the classical equations of motion in the Hamiltonian formalism:

$$\begin{aligned} \dot{x} &= \frac{\partial H}{\partial p} \\ \dot{p} &= -\frac{\partial H}{\partial q}. \end{aligned} \quad \text{.....} \quad (44)$$

Solution of the Schrödinger equation.

Energy eigenkets :

Schrödinger equation allows us to calculate $|\Psi(t)\rangle$ at some instant t given $|\Psi(t_0)\rangle$ at an earlier instant. Equivalently, from the Schrödinger equation we can derive a time evolution operator $\hat{T}(t, t_0)$ which acting on $|\Psi(t_0)\rangle$ gives $|\Psi(t)\rangle$. To be able to evaluate the effect of the time-evolution operator on a general initial ket $|\Psi(t_0)\rangle$ we must first know how it acts on the basis kets used in expanding $|\Psi(t_0)\rangle$. The analysis simplifies if the basis kets are energy eigenkets. Let us write the energy eigenkets as

$$|E_n, a\rangle$$

where a are eigenvalues of observables compatible with $\hat{H}$, i.e., observables whose operators commute with $\hat{H}$. We have

$$\hat{H}\,|E_n, a\rangle = E_n\,|E_n, a\rangle \quad \cdots\cdots (45).$$

We can now expand the time-evolution operator for a conservative system (i.e., $\hat{H}$ is independent of ~~the~~ time)

$$\hat{T}(t, t_0) = e^{-i\hat{H}(t-t_0)/\hbar}$$

in terms of energy eigenkets. We have, taking $t_0 = 0$ for simplicity

$$e^{-i\hat{H}t/\hbar}$$

$$= \sum_{na}{}' \sum_{n'a'} |E_{n'} a'\rangle\langle E_{n'} a'|\, e^{-i\hat{H}t/\hbar}\, |E_n a\rangle\langle E_n a|$$

$$= \sum_{na} |E_n, a\rangle\, e^{-iE_n t/\hbar} \langle E_n a| \quad \cdots\cdots (46)$$

where we have used the orthonormality of the energy eigenkets:

$$\langle E_n, a|E_{n'}, a'\rangle = \delta_{nn'}\,\delta_{aa'}. \quad \cdots\cdots (47)$$

The time evolution operator expanded in this form enables us to solve any initial value problem once the expansion of the initial state ket in terms of the basis energy eigenkets is known. As an example, suppose that the initial state ket expansion reads

$$|\psi(t=0)\rangle = \sum_{n,a} |E_n, a\rangle\langle E_n, a|\psi(0)\rangle$$

$$= \sum_{n,a} C_{na}(0)\, |E_n, a\rangle \,, \qquad (48)$$

then we have

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}\, |\psi(0)\rangle$$

$$= \sum_{n,a} C_{na}(0)\, e^{-iE_n t/\hbar}\, |E_n, a\rangle \,. \qquad (49)$$

In other words, the expansion coefficients change with time as

$$C_{na}(0) \longrightarrow C_{na}(t) = C_{na}(0)\, e^{-iE_n t/\hbar} \,. \qquad (50)$$

Note that this expression is true only when the basis set of states are the energy eigenkets.

Summary:

When $\hat{H}$ does not depend explicitly on time, to find $|\psi(t)\rangle$, given $|\psi(0)\rangle$, proceed as follows:

1. Expand $|\psi(t=0)\rangle$ in terms of eigenkets of $\hat{H}$ which form a basis:

$$|\psi(t=0)\rangle = \sum_{na} c_{na}(0)\, |E_n, a\rangle$$

$$c_{na}(0) = \langle E_n a | \psi(0)\rangle$$

2. Now to obtain $|\psi(t)\rangle$ for arbitrary t, multiply each coefficient $c_{na}(0)$ by $e^{-iE_nt/\hbar}$, where E_n is the eigenvalue of $\hat{H}$ associated with the ket $|E_n, a\rangle$. Thus

$$|\psi(t)\rangle = \sum_{na} c_{na}(0)\, e^{-iE_nt/\hbar}\, |E_n a\rangle .$$

- Stationary states

An important special case is when $|\psi(t=0)\rangle$ is itself an eigenstate of $\hat{H}$. The expansion of $|\psi(t=0)\rangle$ then involves only eigenstates of $\hat{H}$ with the same eigenvalue (for example E_n):

$$|\psi(t=0)\rangle = \sum_a C_{na}(0)\,|E_n a\rangle . \tag{51}$$

In this formula there is no summation over n.

Thus we obtain

$$\begin{aligned}|\psi(t)\rangle &= \sum_a C_{na}(0)\, e^{-iE_n t/\hbar}\,|E_n a\rangle \\ &= e^{-iE_n t/\hbar} \sum_a{}' C_{na}(0)\,|E_n a\rangle \\ &= e^{-iE_n t/\hbar}\,|\psi(t=0)\rangle \end{aligned} \tag{52}$$

The states $|\psi(t)\rangle$ and $|\psi(t=0)\rangle$ therefore differ only by the global phase factor $e^{-iE_n t/\hbar}$

and so these two states are physically indistinguishable. From this we conclude that all physical properties of a system whose state ket is an eigenket of $\hat{H}$ do not vary with time. The eigenstates of $\hat{H}$ are therefore called stationary states.

Energy-time uncertainty relation.

Read Griffiths.

The position-momentum ~~uncertainty~~ ~~are~~ uncertainty relation is often ~~as~~ written in the form

$$\Delta x \, \Delta p \gtrsim \frac{\hbar}{2} \quad \text{- - - - - - - (53)}$$

Equation (53) is often paired with the energy-time uncertainty relation

$$\Delta t \, \Delta E \gtrsim \frac{\hbar}{2} \quad \text{- - - - - - - (54)}$$

The meaning of Δt is quite different from Δx, Δp or ΔE. In non-relativistic quantum mechanics, position, momentum and energy are all dynamical variables – measurable characteristics of the system at any given time. Δx, Δp and ΔE are the uncertainties in the measurements of the variables x, p and E at a particular moment in time.

Time, unlike position, momentum or energy, is not a dynamical variable of the system.

There is nothing called 'time' of a system. Time is an independent variable or a parameter, of which the dynamical variables are functions. In particular, the Δt in the energy-time uncertainty principle is not the standard deviation (i.e., the uncertainty) of a collection of time measurements. It turns out that it is the time taken by the system to change substantially.

We have to make precise what we mean by the phrase 'change substantially'. To do this we consider an observable of the system with operator $\hat{A}$ which does not commute with the Hamiltonian. We have seen previously that the time variation of the expectation value of such an operator is given by

$$i\hbar \frac{d}{dt}\langle A\rangle(t) = \langle [A, H] \rangle \quad \cdots\cdots (55)$$

We can now define a time scale for 'substantial' change of the system as the time required for $\langle A \rangle$ to vary by an amount equal to the uncertainty ΔA of A. Calling the time Δt, we have by definition,

$$\Delta t = \frac{\Delta A}{\left|\frac{d}{dt}\langle A\rangle\right|} = \frac{(\Delta A)\,\hbar}{\langle |[\hat{A}, \hat{H}]| \rangle} \quad \cdots (56)$$

where we have used Eq. (55). We can write Eq. (56) as

$$\Delta A = \cancel{\frac{\Delta t\,|[A, H]|}{\hbar}} = \frac{\Delta t\,|\langle [A, H]\rangle|}{\hbar} \quad \cdots (57).$$

Now, for any two observables A and B, we have

$$\Delta A \cdot \Delta B = \frac{1}{2}\,|\langle [A, B] \rangle|$$

$$\Delta t \equiv \frac{\Delta A}{\left|\frac{d\langle A\rangle}{dt}\right|} \quad \cdots\cdots (56)$$

Substituting $\frac{d\langle A\rangle}{dt}$ from Eq.(55) into Eq.(56) we have

$$\Delta t = \frac{\hbar\,\Delta A}{|\langle[A,H]\rangle|}$$

or,

$$\Delta A = \frac{|\langle[A,H]\rangle|\,\Delta t}{\hbar} \quad \cdots\cdots (57)$$

Now, for any two observables A and B we have

$$\Delta A \cdot \Delta B \geqslant \frac{1}{2}\left|\langle[A,B]\rangle\right|$$

Taking $\hat{B} = \hat{H}$, we have

$$\Delta A \cdot \Delta E \geqslant \frac{1}{2}\left|\langle[\hat{A},\hat{H}]\rangle\right|$$

or, substituting from Eq.(57) into the above equation,

$$\frac{|\langle[A,H]\rangle|\,\Delta t}{\hbar} \cdot \Delta E \geqslant \frac{1}{2}\left|\langle[A,H]\rangle\right|$$

i.e.,

$$\boxed{\Delta t \,.\, \Delta E \geqslant \tfrac{1}{2}\hbar} \qquad \text{- - - - - - (58)}$$

Here Δt depends entirely on what observable A one cares to look at - the change might be rapid for one observable and slow for another. But if ΔE is small, then the rate of change of all observables must be very gradual. To put it the other way round, if any observable changes rapidly, the uncertainty in the energy must be large.

In the extreme case of a stationary state, for which the energy is uniquely determined, all expectation values are constant in time, so that $\Delta t \to \infty$. Thus $\Delta E = 0$ implies that $\Delta t = \infty$.

Ex In the extreme case of a stationary state (i.e., a state with definite energy), expectation values of all operators are constant in time so that

$$\Delta E = 0 \xrightarrow{\text{implies}} \Delta t = \infty$$

To make something happen you must take a linear combination of at least two stationary states, say

$$\Psi(x,t) = a\,\psi_1(x)\,e^{-iE_1t/\hbar} + b\,\psi_2(x)\,e^{-iE_2t/\hbar}$$

where a, b, ψ_1 and ψ_2 are real;

$$|\Psi(x,t)|^2 = a^2\psi_1^2(x) + b^2\psi_2^2(x) + 2ab\,\psi_1(x)\psi_2(x)\cos\left(\frac{E_2-E_1}{\hbar}t\right)$$

Roughly speaking, the position probability density would change ~~would change~~ appreciably ~~if~~ within a time interval of Δt, if the phase of ~~the~~ the cosine function changes by about π during this time, i.e., if

$$\frac{|E_2 - E_1| \Delta t}{\hbar} \approx \pi$$

Roughly $\Delta E = E_2 - E_1$. Therefore

$$\Delta E \Delta t \approx \pi \hbar > \hbar/2 .$$

Conservation of probability, probability current density and equation of continuity.

Shankar, sec 5.3

As a prelude to our study of continuity equation in quantum mechanics, let us recall the analogous equation from electromagnetism. We know in this case that the total charge in the universe is conserved, that is

$$Q(t) = \text{constant, independent of time } t. \quad (1)$$

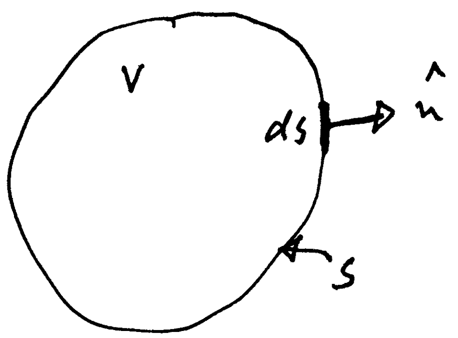
This is an example of a global conservation law, for it refers to the total charge in the universe. But charge is also conserved locally, a fact usually expressed in the form of the continuity equation

$$\frac{\partial \rho(\vec{r},t)}{\partial t} = - \vec{\nabla}.\vec{J} \quad \cdots\cdots (2)$$

where ρ and $\vec{J}$ are the charge and current densities respectively. By integrating this equation over a volume V bounded by a surface S, we get upon invoking Gauss's law

$$\frac{d}{dt}\int_V \rho(\vec{r},t)\, d^3r = -\int_V \vec{\nabla}\cdot\vec{J}\, d^3r$$

$$= -\int_S \vec{J}\cdot d\vec{s}\,. \qquad \cdots\cdots (3)$$



Here $d\vec{s} = ds\,\hat{n}$ where $\hat{n}$ is the outward drawn normal to the surface element ds. Eq.(3) states that any decrease in charge in the volume V is accounted for by the flow of charge out of it, that is to say, charge is not created or destroyed in any volume.

In quantum mechanics, the quantity that is globally conserved is the total probability for finding the particle anywhere in the Universe. We can get this result by expressing the invariance of the norm in the coordinate basis. Since

$$\langle \psi(t) | \psi(t) \rangle = \langle \psi(0) | T^{\dagger}(t)\, T(t) | \psi(0) \rangle$$

$$= \langle \psi(0) | \psi(0) \rangle$$

then

$$\text{constant} = \langle \psi(t) | \psi(t) \rangle$$

$$= \int d^3r \, \langle \psi(t) | \vec{r} \rangle \langle \vec{r} | \psi(t) \rangle$$

$$= \int d^3r \; \psi^*(\vec{r}, t)\, \psi(\vec{r}, t)$$

$$= \int P(\vec{r}, t)\, d^3r \qquad \cdots\cdots \quad (4)$$

where $\vec{P}(\vec{r}, t)$ is the probability density.

This global conservation law for the conservation of probability is analogous to the global conservation law for electric charge (Eq. (1)). To get the equation of continuity for probability we turn to the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \quad \cdots\cdots (5)$$

and its complex conjugate

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*, \quad \cdots\cdots (6)$$

Note that V has to be real, if H is to be hermitian. Multiplying the first of these two equations by ψ^* and the second by ψ, and taking the difference we get

$$i\hbar \frac{\partial}{\partial t}(\psi^* \psi) = -\frac{\hbar^2}{2m}\left(\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*\right)$$

or $$\frac{\partial P}{\partial t} = -\frac{\hbar}{2mi}\vec{\nabla}\cdot\left(\psi^* \vec{\nabla}\psi - \psi \vec{\nabla}\psi^*\right)$$

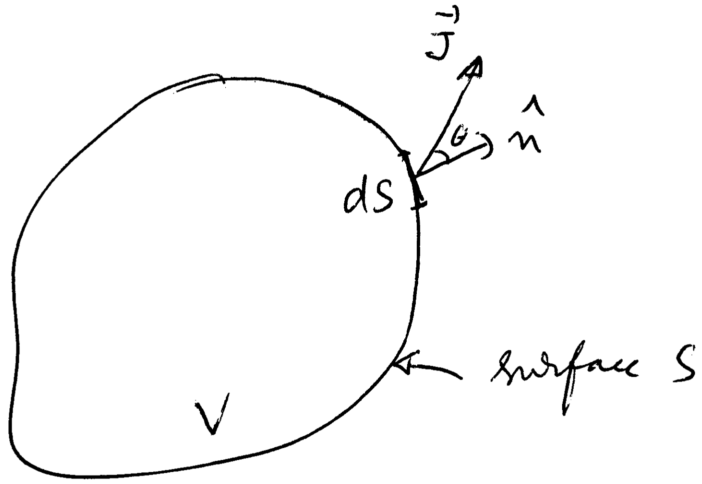
or $$\boxed{\frac{\partial P}{\partial t} = -\vec{\nabla}\cdot\vec{J}} \quad \cdots\cdots\cdots (7)$$

where

$$\vec{J} = \frac{\hbar}{2mi}\left(\psi^* \vec{\nabla}\psi - \psi \vec{\nabla}\psi^*\right) \quad \cdots (8)$$

is the probability current density, that is to say probability flow per unit time per unit area perpendicular to $\vec{J}$.

To get a physical understanding of the equation of continuity for probability, we integrate Eq. (7) over a volume V



$$\int_V \frac{\partial P(\vec{r},t)}{\partial t} d^3r = -\int_V \vec{\nabla}\cdot\vec{J}\, d^3r$$

or $$\frac{d}{dt}\int_V P(\vec{r},t)\,d^3r = -\oint_S \vec{J}\cdot d\vec{s} \quad \cdots\cdots (9)$$

Now $\int_V P(\vec{r},t)\,d^3r$ is the probability of finding the particle in the volume V. Next,

$$\vec{J}\cdot\vec{ds} = J\cos\theta\, ds = J_{\perp}\, ds$$

where $J_{\perp}$ is the component of $\vec{J}$ along the outward drawn normal of the surface element ds. $\vec{J}\cdot\vec{ds}$ gives the probability per unit time that the particle would move out of the volume through ds. Therefore $\oint_S \vec{J}\cdot\vec{ds}$ is the probability that the particle would move out of the volume in unit time.

Thus, Eq (9) tells us that any decrease in the probability of finding the particle in the volume V is due to the fact that there exists a probability for the particle to move out of the volume through the bounding surface S.

Other pictures of quantum dynamics:

In the Schrödinger picture discussed so far, it is the time-independent operators which correspond to observables of the system. The evolution of the system is entirely contained in the state vector $|\psi(t)\rangle$.

The possibility of formulating quantum dynamics in alternative ways arises because the mathematical entities such as state vectors and operators are not the quantities which are ~~not the quantities which are~~ directly accessible to physical measurement. Rather, the comparison with observation is made in terms of eigenvalues and of expansion coefficients which are scalar products in the Hilbert space. Measuring an observable A means finding one of its eigenvalues A′, the probability of this particular result being given by $|\langle A'|\Psi\rangle|^2$ if $|\Psi\rangle$ denotes the state of the system, the average value of the measurement being given by $\langle\Psi|\hat{A}|\Psi\rangle$. It follows that any formulation of quantum mechanics is equally acceptable as the Schrödinger picture if in the new picture:

(a) the operators corresponding to observables have the same eigenvalue spectrum as in the Schrödinger picture, and if

(b) the scalar products of states and expectation values of operators in the new picture is the same as in the Schrödinger picture.

These conditions are met if we transform all vectors (state vector, base vectors) and all operators in the Schrödinger picture by ~~an operator~~ a unitary operator U in the following manner:

$$|\bar{a}\rangle = U|a\rangle, \quad \text{i.e.,} \quad \langle\bar{a}| = \langle a|U^{+} \qquad (1)$$

and

$$\bar{A} = UAU^{+}. \qquad \ldots\ldots \qquad (2).$$

A bar over the vectors and operators ~~will~~ denotes the respective quantities in the new picture. Equations (1) and (2) are called unitary or canonical ~~transf~~ transformations.

For the eigenvalue equation

$$A|A'\rangle = A'|A'\rangle$$

we obtain

$$UAU^{+}U|A'\rangle = A'U|A'\rangle$$

or

$$\bar{A}\,|\overline{A'}\rangle = A'\,|\overline{A'}\rangle, \qquad \ldots\ldots \qquad (3)$$

This equation shows that eigenvalues of $\bar{A}$ are the same as those of A in agreement with condition (a). Eigenvectors of $\bar{A}$ are ~~however~~ different from those of A.

The eigenvectors change from $|A'\rangle$ to $\overline{|A'\rangle} = U|A'\rangle$.

Condition (b) is also satisfied if U is a unitary operator. Thus

$$\overline{\langle a'|b'\rangle} = \langle a'|U^{\dagger}U|b'\rangle = \langle a'|b'\rangle$$

since $U^{\dagger}U = UU^{\dagger} = \hat{1}$. Further,

$$\langle\psi|A|\psi\rangle = \langle\underset{\sim}{\psi|U^{\dagger}}\underset{\sim}{UAU^{\dagger}}\underset{\sim}{U|\psi}\rangle$$

$$= \langle\bar{\psi}|\bar{A}|\bar{\psi}\rangle \quad \text{------} \quad (4)$$

Hence scalar products and expectation values are unchanged under a unitary transformation.

Infinitely many different choices of U are possible leading to different pictures of quantum mechanics. Of the many possible pictures, Heisenberg picture and the interaction picture are the most useful in the study of quantum dynamics.

Heisenberg picture.

The Heisenberg picture is obtained if we choose ~~for~~ U at time t to be the inverse of the unitary time evolution operator $T(t, t_0)$ of the state vectors in the Schrödinger picture. Thus

$$U(t) = [T(t, t_0)]^{-1} = T^{+}(t, t_0) = T(t_0, t). \quad \text{-- (5)}$$

Hence, in the Heisenberg picture, the state vector of the system and the operators are

$$|\psi_H(t)\rangle = U(t)|\psi_S(t)\rangle = T^{+}(t, t_0)|\psi_S(t)\rangle \quad \text{---(6)}$$

and

$$A_H(t) = U(t) A_S U^{+}(t) = T^{+}(t, t_0) A_S T(t, t_0), \quad \text{--(7)}$$

where we have used the subscripts S and H to distinguish between the Schrödinger picture and the Heisenberg picture.

From Eq. (6) we ~~obtai~~ obtain

$$
\begin{aligned}
|\Psi_H(t)\rangle &= T^{-1}(t,t_0)\,|\Psi_S(t)\rangle \\
&= T^{-1}(t,t_0)\,T(t,t_0)\,|\Psi_S(t_0)\rangle \\
&= |\Psi_S(t_0)\rangle. \qquad \cdots\cdots (8)
\end{aligned}
$$

We thus see that in the Heisenberg picture, the state vector $|\Psi_H(t)\rangle$ does not change with time at all, ~~its value~~ The state ket in the Heisenberg picture is equal to the initial state ket in the Schrödinger picture. Therefore we will write the state vector in the Heisenberg picture simply as $|\Psi_H\rangle$:

$$
|\Psi_H\rangle = |\Psi_S(t_0)\rangle. \qquad \cdots\cdots (9)
$$

In the Heisenberg picture the operators $A_H(t)$, on the other hand, are time-dependent.

By differentiating Eq. (7) we find

$$\frac{d}{dt} A_H(t) = \left[\frac{\partial}{\partial t} T^+(t,t_0)\right] A_s(t)\, T(t,t_0)$$

$$+ \; T^+(t,t_0) \frac{dA_s(t)}{dt} T(t,t_0)$$

$$+ \; T^+(t,t_0) A_s(t) \left[\frac{\partial}{\partial t} T(t,t_0)\right]$$

where we have allowed for the possibility that even in the Schrödinger picture, some operators may depend on time explicitly. To continue, we use the differential equations for $T(t,t_0)$ and $T^+(t,t_0)$:

$$\left.\begin{aligned} & i\hbar \frac{\partial}{\partial t} T(t,t_0) = H_s(t)\, T(t,t_0) \\ & \text{i.e.,} \\ & -i\hbar \frac{\partial}{\partial t} T^+(t,t_0) = T^+(t,t_0)\, H_s(t) \end{aligned}\right\} \cdots\cdots (10)$$

Using Eqs. (10) we obtain

$$i\hbar \frac{dA_H(t)}{dt} = -T^{\dagger}(t,t_0)\, H_S(t)\, A_S(t)\, T(t,t_0)$$
$$+\ T^{\dagger}(t,t_0)\, A_S(t)\, H_S(t)\, T(t,t_0)$$
$$+\ i\hbar\ T^{\dagger}(t,t_0)\, \frac{dA_S(t)}{dt}\, T(t,t_0)\, .$$

In the first and the second terms of this equation let us insert between A_S and H_S the product $T(t,t_0)T^{\dagger}(t,t_0)$, which is equal to the identity operator. We get

$$i\hbar \frac{dA_H(t)}{dt} = -T^{\dagger}(t,t_0)\, H_S(t)\, \underbrace{T(t,t_0)\, T^{\dagger}(t,t_0)}_{\hat{1}}\, A_S(t)\, T(t,t_0)$$
$$+\ T^{\dagger}(t,t_0)\, A_S(t)\, T(t,t_0)\, T^{\dagger}(t,t_0)\, H_S(t)\, T(t,t_0)$$
$$+\ i\hbar\ T^{\dagger}(t,t_0)\, \frac{dA_S}{dt}\, T(t,t_0)\, .$$

According to definition (7), we obtain

$$i\hbar \frac{dA_H(t)}{dt} = -H_H(t)\, A_H(t) + A_H(t)\, H_H(t)$$
$$+\ i\hbar \left(\frac{dA_S}{dt}\right)_H$$

or,

$$i\hbar \frac{dA_H(t)}{dt} = \left[A_H(t), H_H(t)\right] + i\hbar\left(\frac{dA_S(t)}{dt}\right)_H . \quad \text{---(11)}$$

If we have a conservative system, i.e., if H_S in the Schrödinger picture is independent of t, then (with $H_S \equiv H$),

$$H_H(t) = e^{iH(t-t_0)/\hbar}\, H\, e^{-iH(t-t_0)/\hbar} = H \quad \text{---(12)}$$

i.e., the Hamiltonian in the Heisenberg picture is also independent of time and is the same as that in the Schrödinger picture. Furthermore, if A_S is independent of time in the Schrödinger picture, the equation of motion, Eq. (11), simplifies to

$$i\hbar \frac{dA_H(t)}{dt} = \left[A_H(t), H\right], \quad \text{------(13)}$$

Eqs. (11) and (13) are known as the Heisenberg equation of motion. They are analogous to the classical equations of motion expressed in terms of Poisson brackets. In classical mechanics if $F = F(q(t), p(t))$ is a dynamical variable which does not depend upon time explicitly, then the equation of motion for F can be written as

$$\frac{dF}{dt} = \{F, H\}_{PB}$$

Thus, transition from classical mechanics to quantum mechanics in the Heisenberg picture can be made by the formal replacement

$$\{F, H\}_{PB} \longrightarrow \frac{1}{i\hbar}[\hat{F}, \hat{H}].$$

Base kets in the Heisenberg picture.

So far we have avoided asking how the base kets evolve in time. A common misconception is that as time goes on, all kets move in the Schrödinger picture and are stationary in the Heisenberg picture. This is not the case as we will make clear shortly. The important point is to distinguish the behaviour of state kets from that of base kets.

The base kets are eigenkets of an observable (or a set of compatible observables):

$$\hat{A}|a'\rangle = a'|a'\rangle. \quad \text{------} \quad (14)$$

In the Schrödinger picture $\hat{A}$ does not change, so that the base kets must remain unchanged. Unlike state kets, the base kets <u>do not</u> change in the Schrödinger picture.

The whole situation is very different in the Heisenberg picture. In the Heisenberg picture, the base kets are

$$|a', t\rangle_H = U(t)\,|a'\rangle$$
$$= T^{+}(t, t_0)\,|a'\rangle, \quad \cdots\cdots (15)$$

i.e., the base kets in the Heisenberg picture change with time. Because of the appearance of $T^{+}(t, t_0)$ rather than $T(t, t_0)$ in Eq. (15), the Heisenberg picture base kets are seen to 'rotate' oppositely in the Hilbert space when compared with the Schrödinger picture state kets. Specifically, the Heisenberg picture base kets $|a', t\rangle_H$ satisfy the 'wrong sign' Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |a', t\rangle_H = -H\,|a', t\rangle_H \quad \cdots\cdots (16)$$

which is similar to the equation of motion of the state kets in the Schrödinger picture, except for the all-important minus sign. Its appearance shows that, if in the Schrödinger picture we regard the state vectors as 'rotating' in a certain sense in the abstract Hilbert space and operators with their eigenvectors as fixed, then in the Heisenberg picture the state vectors stand still and the operators with their eigenvectors 'rotate' in the opposite direction. This is summarized in Table 1 below.

Table 1 : The Schrödinger picture versus the Heisenberg picture.

	Schrödinger picture	Heisenberg picture
State ket	Moving	Stationary
Observable	Stationary	Moving
Base kets	Stationary	Moving oppositely to state kets in Schrödinger picture.

Transition amplitude.

Transition amplitudes play an important role in quantum mechanics. Suppose there is a physical system prepared at $t=0$ to be in an eigenstate of observable A with eigenvalue a'. At some later time t, we may ask what is the probability amplitude ~~that~~ for the system to be found in an eigenstate of observable B with eigenvalue b'? This probability amplitude is also called the transition amplitude.

In the Schrödinger picture, the state ket at t is given by

$$|\psi_S(t)\rangle = T(t,t_0)|a'\rangle$$

while the base kets do not vary with time.

So the transition amplitude is

$$\langle b' | \Psi_S(t) \rangle = \underbrace{\langle b'}_{\text{base bra in SP}^{+}} | \underbrace{T(t,t_0) | a' \rangle}_{\text{state ket in SP}} \quad \cdots (17)$$

In contrast, in the Heisenberg picture, the state ket is stationary, that is, it remains as $|a'\rangle$ at all times, but the base bra evolves oppositely. So the transition amplitude is

$$\langle b' t | a' \rangle_H = \underbrace{\langle b' | T(t,t_0)}_{\text{base bra in HP}^{*}} \cdot \underbrace{|a'\rangle}_{\text{state ket in HP}} \quad \cdots (18)$$

Obviously (17) and (18) are the same and they both can be written as

$$\langle b' | T(t,t_0) | a' \rangle .$$

$^{+}$ SP for Schrödinger picture

* HP for Heisenberg picture

Examples of Heisenberg equation of motion for operators:

Generally, Heisenberg equations of motion are more difficult to solve than the corresponding classical equations because of the lack of commutivity of quantum mechanical operators.

First, let us assume that the Schrödinger picture Hamiltonian is independent of time and is of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{\vec{r}}). \quad \cdots\cdots (19)$$

Because $\hat{H}$ is independent of time, we can write it as

$$\hat{H} = \hat{H}_H(t) = \frac{\hat{\vec{P}}_H^{\,2}(t)}{2m} + V(\hat{\vec{r}}_H(t)). \quad \cdots (20)$$

From now on we will dispense with the subscript 'H' to represent Heisenberg picture operators.

The Heisenberg picture operator $\vec{r}(t)$ in three-dimensions obeys the equation of motion

$$i\hbar \frac{d\vec{r}(t)}{dt} = \left[\vec{r}(t), H_H\right] . \quad \text{- - - - -} \quad (21)$$

In the commutator of Eq. (21), $\vec{r}(t)$ commutes with $V(\vec{r}(t))$, since an operator always commutes with a function of itself. However, $\vec{r}(t)$ fails to commute with $\vec{P}^2(t)/2m$. To evaluate their commutator, let us notice that, by components

$$\left[r_i(t), p_j(t)\right] = r_i(t)\,p_j(t) - p_j(t)\,r_i(t)$$

$$= U r_i U^{+} U p_j U^{+} - U p_j U^{+} U r_i U^{+}$$

$$= U r_i p_j U^{+} - U p_j r_i U^{+}$$

$$= U\,(r_i p_j - p_j r_i)\,U^{+}$$

$$= U\,(i\hbar\,\delta_{ij}\,\hat{\mathbb{1}})\,U^{+}$$

$$= i\hbar\,\delta_{ij}\,\hat{\mathbb{1}} \quad \text{- - - - - - - -} \quad (22)$$

Here U
$= T^{+}(t,0)$
$= e^{iHt/\hbar}$

Thus $\vec{r}(t)$ and $\vec{p}(t)$ in the Heisenberg picture obey the same commutation relation as $\vec{r}$ and $\vec{p}$ in the Schrödinger picture.

By a simple calculation we find

$$\left[\vec{r}(t), \frac{\vec{p}^{\,2}(t)}{2m} \right] = \frac{i\hbar}{m} \vec{p}(t) \qquad \cdots\cdots (23)$$

So That

$$\boxed{\frac{d\vec{r}(t)}{dt} = \frac{\vec{p}(t)}{m}} \;. \qquad \cdots\cdots (24)$$

The position operator in the Heisenberg picture obeys the usual classical equation.

Next, let us work out the equation of motion for $\vec{p}(t)$. We have

$$i\hbar \frac{d\vec{p}(t)}{dt} = \left[\vec{p}(t), H_H \right]$$

Now $\vec{p}(t)$ commutes with the kinetic energy part $p^2(t)/2m$ of H. We must evaluate

$$[\vec{p}(t), V(\vec{r}(t))]$$

$$= U\,[\vec{p}, V(\vec{r})]\,U^{+} \qquad \left|\begin{array}{l} U = T^{+}(t,0) \\ \quad = e^{iHt/\hbar} \end{array}\right.$$

But

$$[\vec{p}, V(\vec{r})] = -i\hbar\,\vec{\nabla} V(\vec{r})$$

~~so that~~

$$\cancel{[\vec{p}, V(\vec{r})] = -i\hbar\,\vec{\nabla} V(\vec{r})}$$

so that

$$[\vec{p}(t), V(\vec{r}(t))]$$

$$= -i\hbar\; U\,\vec{\nabla} V(\vec{r})\,U^{+}$$

$$= -i\hbar\; e^{iHt/\hbar}\,\vec{\nabla} V(\vec{r})\,e^{-iHt/\hbar}$$

$$= -i\hbar\; \vec{\nabla}_{\vec{r}(t)} V(\vec{r}(t)).$$

Hence $\vec{p}(t)$ obeys the equation of motion

$$\frac{d\vec{p}(t)}{dt} = -\vec{\nabla}_{\vec{r}(t)} V(\vec{r}(t)) \quad \cdots\cdots \quad (25)$$

Again this is the usual classical equation of motion. We can interpret $-\vec{\nabla}_{\vec{r}(t)} V(\vec{r}(t))$ as the operator for the force on the particle.

We will now consider a ~~few~~ few special cases in which the Heisenberg equation of motion for the operators are easy to solve.

(a) Free particle.

For a free particle (i.e., $V(\vec{r}) = 0$), the Heisenberg equation of motion for $\vec{p}(t)$ is

$$\frac{d\vec{p}(t)}{dt} = 0 \quad \cdots\cdots\cdots \quad (26)$$

Thus, the momentum operator for a free particle is a constant of motion; i.e.,

$$\vec{p}(t) = \vec{p}(0) .$$

The equation of motion for the position operator is then

$$\frac{d\vec{r}(t)}{dt} = \frac{\vec{p}(t)}{m} = \frac{\vec{p}(0)}{m}$$

i.e.,
$$\vec{r}(t) = \vec{r}(0) + \frac{\vec{p}(0)}{m} t , \quad \cdots\cdots (27)$$

If $|\psi(0)\rangle$ is the wavepacket of the particle at $t=0$, then the center of the wave packet $\langle \vec{r} \rangle_t$ is given by

$$\cancel{\langle \vec{r} \rangle_t = \langle \vec{r} \rangle_0 + \frac{\vec{p}(0)}{m} t . \quad \cdots\cdots (28)}$$

$$\langle \vec{r} \rangle_t = \langle \vec{r} \rangle_0 + \frac{\langle \vec{p} \rangle_0}{m} t , \quad \cdots\cdots (28)$$

a familiar result.

(6) Harmonic oscillator

The Hamiltonian for a one-dimensional harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 . \quad \text{------} \ (29)$$

Since H is independent of time, H must be the same both in the Schrödinger and the Heisenberg picture, i.e.,

$$H = H(t) = \frac{p^2(t)}{2m} + \frac{1}{2} m\omega^2 x^2(t) \quad \text{----} \ (30)$$

The Heisenberg equation of motion for $x(t)$ is

$$i\hbar \frac{dx(t)}{dt} = [x(t), H_H]$$

i.e.,

$$\frac{dx(t)}{dt} = \frac{p(t)}{m} \quad \text{--------} \ (31).$$

The equation of motion for $p(t)$ is

$$\frac{dp(t)}{dt} = -\frac{\partial}{\partial x(t)}\left(\frac{1}{2} m\omega^2 x^2(t)\right)$$

or

$$\frac{dp(t)}{dt} = -m\omega^2 x(t) \quad \text{-------} \ (32).$$

From Eqs. (31) and (32) we obtain

$$\frac{d^2 x(t)}{dt^2} + \omega^2 x(t) = 0 \quad \cdots\cdots\cdots (33)$$

$$\frac{d^2 p(t)}{dt^2} + \omega^2 p(t) = 0 \, . \quad \cdots\cdots\cdots (34)$$

The solutions of $\hat{x}(t)$ and $\hat{p}(t)$ are:

$$\hat{x}(t) = \hat{A} \cos \omega t + \hat{B} \sin \omega t \quad \cdots\cdots (35)$$

$$\hat{p}(t) = \hat{C} \cos \omega t + \hat{D} \sin \omega t \quad \cdots\cdots (36)$$

where A, B, C and D are operators independent of time. To find A and B we use the initial conditions

$$x(t)\Big|_{t=0} = x(0)$$

and

$$\frac{dx}{dt}\Big|_{t=0} = \frac{p(0)}{m} \, .$$

We find

$$\left.\begin{aligned} A &= x(0) \\ B &= \frac{p(0)}{m\omega} \end{aligned}\right\} \quad \cdots\cdots\cdots (37).$$

Similarly, to find C and D, we use the initial conditions

$$p(t)\Big|_{t=0} = p(0)$$

$$\frac{dp(t)}{dt}\Big|_{t=0} = -m\omega^2 x(0)$$

We obtain

$$C = p(0) \text{ and } D = -m\omega x(0). \quad \text{----} (38)$$

Hence, finally

$$x(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t \quad \text{----} (39)$$

$$p(t) = p(0)\cos\omega t - m\omega x(0)\sin\omega t. \quad \text{----} (40)$$

Equations (39) and (40) are the full solutions of $x(t)$ and $p(t)$ for a one-dimensional harmonic oscillator.

- Equation of motion for the creation and destruction operators

For an one-dimensional harmonic oscillator,

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$$

$$= \left(a^{\dagger} a + \frac{1}{2} \right) \hbar \omega \quad \cdots\cdots (41)$$

where

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{ip}{m\omega} \right) \quad \cdots\cdots (42)$$

$$a^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{ip}{m\omega} \right) \quad \cdots\cdots (43)$$

We have

$$[a, a^{\dagger}] = 1$$

$$[H, a] = - a \hbar \omega$$

$$[H, a^{\dagger}] = a^{\dagger} \hbar \omega$$

Since H is independent of time

$$H = H(t) = \left(a^{\dagger}(t) a(t) + \frac{1}{2} \right) \hbar \omega$$

The equations of motion for $a(t)$ and $a^+(t)$ are

$$i\hbar \frac{da(t)}{dt} = [a(t), H] = a(t)\hbar\omega$$

$$i\hbar \frac{da^+(t)}{dt} = [a^+(t), H] = -a^+(t)\hbar\omega,$$

i.e.,

$$\frac{da(t)}{dt} = -i\omega a(t)$$

$$\frac{da^+(t)}{dt} = i\omega a^+(t).$$

These equations have simple solutions

$$a(t) = a(0) e^{-i\omega t}$$

$$a^+(t) = a^+(0) e^{i\omega t}.$$

Note: The equations of motion for $a(t)$ and $a^+(t)$ could be found from those for $x(t)$ and $p(t)$. For example,

$$a(t) = \sqrt{\frac{m\omega}{2\hbar}} \left(x(t) + \frac{i\,p(t)}{m\omega} \right)$$

$$\therefore \quad \frac{da(t)}{dt} = \sqrt{\frac{m\omega}{2\hbar}} \left(\frac{dx(t)}{dt} + \frac{i}{m\omega}\frac{dp(t)}{dt} \right)$$

$$= \sqrt{\frac{m\omega}{2\hbar}} \left(\frac{p(t)}{m} - \frac{i}{m\omega} m\omega^2 x(t) \right) = -i\omega a(t).$$

Similarly for $a^+(t)$.

The Interaction Picture or The Dirac Picture.

The picture of quantum dynamics due to Dirac is intermediate between the Schrödinger and the Heisenberg pictures. The interaction picture is useful when we can split the Hamiltonian in the Schrödinger picture in two parts:

$$H = H_0 + V(t) \quad \cdots\cdots (1)$$

where H_0 is the unperturbed Hamiltonian and $V(t)$ is the perturbation Hamiltonian which may depend on time. We define the interaction picture kets and operators by ~~use~~ means of a unitary transformation from the Schrödinger picture using the unitary operator

$$U(t) = e^{i H_0 t/\hbar} . \quad \cdots\cdots (2)$$

$U(t)$ is the inverse of the time evolution operator in the Schrödinger picture if V were absent. (We take $t_0 = 0$, i.e., the initial time is taken to be zero for simplicity).

We write

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar} |\psi_S(t)\rangle \quad \text{------} (3)$$

$$A_I(t) = e^{iH_0 t/\hbar} A_S \, e^{-iH_0 t/\hbar} \quad \text{-----} (4).$$

The operator H_0 is the same in both the Schrödinger and in the ~~Heisenberg~~ interaction pictures:

$$H_{0,I}(t) = e^{iH_0 t/\hbar} H_0 \, e^{-iH_0 t/\hbar}$$

$$= H_0 \, e^{iH_0 t/\hbar} e^{-iH_0 t/\hbar}$$

$$= H_0 \quad \text{------} (5)$$

In the interaction picture both the state vectors and operators are time-dependent. From Eq (3) and Eq (4) we can easily derive the equations of motion for state kets and operators in the interaction picture.

Equation of motion for $|\psi_I(t)\rangle$

Taking the time derivative of Eq. (3) we have

$$i\hbar \frac{d}{dt}|\psi_I(t)\rangle$$

$$= i\hbar\left(\frac{i}{\hbar}\right)e^{iH_0t/\hbar} H_0|\psi_s(t)\rangle + e^{iH_0t/\hbar}\left(i\hbar\frac{d}{dt}|\psi_s(t)\rangle\right)$$

$$= -e^{iH_0t/\hbar} H_0|\psi_s(t)\rangle + e^{iH_0t/\hbar}\left(H_0+V_s(t)\right)|\psi_s(t)\rangle$$

$$= e^{iH_0t/\hbar} V_s(t)|\psi_s(t)\rangle$$

$$= e^{iH_0t/\hbar} V_s(t)\, e^{-iH_0t/\hbar} e^{iH_0t/\hbar}|\psi_s(t)\rangle$$

$$= V_I(t)|\psi_I(t)\rangle$$

i.e
$$\boxed{i\hbar\frac{d}{dt}|\psi_I(t)\rangle = V_I(t)|\psi_I(t)\rangle} \quad \text{----} (6)$$

where
$$V_I(t) = e^{iH_0t/\hbar} V_s(t)\, e^{-iH_0t/\hbar} \quad \text{---} (7)$$

Equation of motion for $A_I(t)$

The operator $A_I(t)$ in the Dirac picture is given by Eq (4):

$$A_I(t) = e^{iH_0 t/\hbar} A_S \, e^{-iH_0 t/\hbar} .$$

We assume that A_S does not depend on time explicitly. From this equation we get

$$\begin{aligned} i\hbar \frac{dA_I(t)}{dt} &= -H_0 \, e^{iH_0 t/\hbar} A_S \, e^{-iH_0 t/\hbar} \\ &\quad + e^{iH_0 t/\hbar} A_S \, e^{-iH_0 t/\hbar} H_0 \\ &= -H_0 A_I(t) + A_I(t) H_0 \\ &= [A_I(t), H_0] = [A_I(t), H_{0I}] \end{aligned}$$

since $H_0 = H_{0I}$. Thus, the equation of motion for $A_I(t)$ is

$$\boxed{i\hbar \frac{dA_I(t)}{dt} = [A_I(t), H_{0I}]} \quad \cdots\cdots (8)$$

Equation (6) shows that the time development of state kets in the interaction picture is governed solely by the interaction Hamiltonian (i.e., perturbation part of the Hamiltonian) expressed in the interaction picture. This is the great advantage of the interaction picture. We can solve for $|\psi_I(t)\rangle$ perturbatively.

Eq. (8) shows that the equation of motion for $A_I(t)$ is determined by H_0 only, i.e., they are equations of motion of the system without interactions. Hence in the Dirac picture the operators obey free equations of motion which is again an advantage because we can solve for $A_I(t)$ exactly.

The Dirac picture is widely used in Quantum field theory.

Dyson series for interaction picture state kets

The time evolution of the interaction picture state ket is given in Eq. (6), which is quoted here:

$$i\hbar \frac{d}{dt}|\psi_I(t)\rangle = V_I(t)\,|\psi_I(t)\rangle \quad \cdots\cdots (6)$$

where

$$|\psi_I(0)\rangle = |\psi_S(0)\rangle \equiv |\psi\rangle \quad \cdots\cdots (9)$$

We can write Eq. (6) as an integral equation in which we incorporate the initial condition (9):

$$|\psi_I(t)\rangle = |\psi_I(0)\rangle + \left(-\frac{i}{\hbar}\right)\int_0^t dt_1\, V_I(t_1)\,|\psi_I(t_1)\rangle\, dt_1 \quad \cdots (10).$$

Iterating this equation once, we get

$$\cancel{|\psi_I(t)\rangle = |\psi_I(0)\rangle + (-i/\hbar)\int_0^t dt\, V(t)\,[\,|\psi_I(0)\rangle}$$

$$|\Psi_I(t)\rangle = |\Psi_I(0)\rangle$$
$$+ (-i/\hbar)\int_0^t dt_1\, V_I(t_1)\left[|\Psi_I(0)\rangle + (-i/\hbar)\int_0^{t_1} dt_2\, V_I(t_2)|\Psi_I(t_2)\rangle\right]$$
$$= |\Psi_I(0)\rangle$$
$$+ (-i/\hbar)\int_0^t dt_1\, V_I(t_1)\, |\Psi_I(0)\rangle$$
$$+ (-i/\hbar)^2 \int_0^t dt_1\, V_I(t_1)\int_0^{t_1} V_I(t_2)\,|\Psi_I(t_2)\rangle\, dt_2$$

This equation is exact. If we continue to iterate this equation indefinitely, we get an infinite series for $|\Psi_I(t)\rangle$ called the Dyson series. We have

$$|\Psi_I(t)\rangle = |\Psi_I(t_0)\rangle + (-i/\hbar)\int_0^t dt_1\, V_I(t_1)\,|\Psi_I(0)\rangle$$
$$+ (-i/\hbar)^2\int_0^t dt_1\int_0^{t_1} dt_2\, V_I(t_1)\, V_I(t_2)\; |\Psi_I(0)\rangle$$
$$+ (-i/\hbar)^3\int_0^t dt_1\int_0^{t_1} dt_2\int_0^{t_2} dt_3\, V_I(t_1)\, V_I(t_2)\, V_I(t_3)\;|\Psi_I(t_0)\rangle$$
$$+ \cdots$$
$$+ (-i/\hbar)^n\int_0^t dt_1\int_0^{t_1} dt_2\cdots\int_0^{t_{n-1}} dt_n\; V_I(t_1)\cdots V_I(t_n)\;|\Psi_I(0)\rangle$$
$$+ \cdots$$

We can write this equation as

$$|\psi_I(t)\rangle = T_I(t)\,|\psi_I(0)\rangle$$

where

$$T_I(t) = \hat{\mathbb{1}} + (-i/\hbar)\int_0^t dt_1\, V_I(t_1)$$
$$+ (-i/\hbar)^2 \int_0^t dt_1 \int_0^{t_1} dt_2\, V_I(t_1)\, V_I(t_2)$$
$$+ (-i/\hbar)^3 \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3\, V_I(t_1)\, V_I(t_2)\, V_I(t_3)$$
$$+ \cdots$$
$$+ (-i/\hbar)^n \int_0^t dt_1 \cdots \int_0^{t_{n-1}} dt_n\, V_I(t_1)\, V_I(t_2) \cdots V_I(t_n)$$
$$+ \cdots$$

or

$$T_I(t) = \hat{\mathbb{1}} + \sum_{n=1}^{\infty} (-i/\hbar)^n \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n\, T\left(V_I(t_1) \cdots V_I(t_n)\right)$$

The operator $T_I(t)$ is the time-evolution operator for the interaction picture state vectors. Now, as we have explained earlier in the context of the time evolution operator in the Schrödinger picture, we can write

$$\int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \; V_I(t_1)\, V_I(t_2) \cdots V_I(t_n)$$

$$= \frac{1}{n!} \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \; T\big(V_I(t_1)\, V_I(t_2) \cdots V_I(t_n)\big) \quad (11)$$

Therefore

$$\boxed{U_I(t) = \hat{\mathbb{1}} + \sum_{n=1}^{\infty} (-i/\hbar)^n \frac{1}{n!} \int_0^t dt_1 \cdots \int_0^t dt_n \; T\big(V_I(t_1) \cdots V_I(t_n)\big)} \quad (12)$$

This is the Dyson formula for the time evolution operator of the state kets in the interaction picture.

Symbolically, we write

$$U_I(t) = T\, e^{-\frac{i}{\hbar}\int_0^t V(t')\,dt'} \qquad \cdots\cdots (13)$$

—— x ——

End