QM-09 Lecture Notes*
Time Development in Quantum Mechanics

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Contents

§1 Time Evolution in Quantum Systems-I

Description of state of a quantum mechanical system at one time is by state vector in the Hilbert space.As the system evolves this state vector will change. General requirements on time evolution lead to time evolution

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governed by unitary operator and for short times by a hermitian operator H which will be identified with Hamiltonian of the system.

Let $|\psi t_0\rangle$ represent the state of system at time t_0 and $|\psi t\rangle$ represent the state at time t. We assume that $|\psi t_0\rangle$ at time t_0 determines the state at time t completely. The principle of superposition should apply at these two times t_0 and t. If we have a relation at time t_0

$$|\psi t_0\rangle = \alpha|\chi t_0\rangle + \beta|\phi t_0\rangle \tag{1}$$

between three possible states,$|\psi\rangle, |\chi\rangle, |\phi\rangle$, the same relation must hold at all times $t > t_0$ when the system is left undisturbed

$$|\psi(t)\rangle = \alpha|\chi t\rangle + \beta|\phi t\rangle \tag{2}$$

Thus if we write

$$|\psi t\rangle = U(t, t_0)|\psi t_0\rangle \qquad \text{etc.} \tag{3}$$

Then $U(t, t_0)$ must be a linear operator independent of ψ. Obviously U must reduce to the identity operator at time $t = t_0$

$$U(t_0, t_0) = I \ . \tag{4}$$

Next we demand that the norm of vector $|\psi t\rangle$ should not change with time and hence

$$\langle\psi t|\psi t\rangle = \langle\psi t_0|\psi t_0\rangle \qquad \text{for all } t \tag{5}$$

The above requirements (2) and (5), respectively, imply that the operator U must be a linear operator and that it must be unitary.

$$UU^\dagger = U^\dagger U = I \tag{6}$$

We shall now derive a differential equation satisfied by the state vector at time t. We, therefore, compute

$$\begin{aligned} \frac{d}{dt}|\psi t\rangle &= \lim_{\Delta t \to 0} \frac{|\psi t + \Delta t)\rangle - |\psi t\rangle}{\Delta t} \\ &= \lim_{\Delta t \to 0} \frac{(U(t + \Delta t, t) - I)}{\Delta t}|\psi t\rangle \qquad (7) \\ \text{or } \frac{d}{dt}|\psi t\rangle &= \hat{X}|\psi t\rangle \qquad (8) \\ \text{where } \hat{X}(t) &= \lim_{\Delta t \to 0} \frac{U(t + \Delta t, t) - I}{\Delta t} \qquad (8") \\ &= \frac{d}{dt'}U(t, t')|_{t'=t} \end{aligned}$$

The operator $\hat{X}$ can be shown to be anti-hermitian and hence with notation $H(t) \equiv X/(i\hbar)$,$H(t)$ will be hermitian. We therefore write Eq.(88) as

$$i\hbar\frac{d}{dt}|\psi t\rangle = \hat{H}(t)|\psi t\rangle \tag{9}$$

where

$$\hat{H}(t) = \frac{1}{i\hbar}\frac{\partial}{\partial t}U(t,t')|_{t'=t} \tag{10}$$

We shall now check that $H(t)$ must be a hermitian operator. Consider Link[1]

$$U^\dagger(t,t')U(t,t') = I \tag{11}$$

Differentiating w.r.t. t we get

$$\left\{\frac{\partial}{\partial t}U^\dagger(t,t')\right\}U(t,t') + U^\dagger\left\{\frac{\partial}{\partial t}U(t,t')\right\} = 0 \tag{12}$$

Setting $t' = t$ and using $U(t,t) = I$ we have

$$\begin{aligned}
\frac{d}{dt}U^\dagger(t,t')|_{t'=t} + \frac{d}{dt}U(t,t')|_{t'=t} &= 0 && (13)\\
\text{or}\qquad (\frac{1}{i\hbar}\hat{H})^\dagger + \frac{1}{i\hbar}\hat{H}) &= 0 && (14)\\
\text{or}\qquad -i\hat{H}^\dagger + \hat{H} &= 0 && (15)\\
\text{or}\qquad \hat{H}^\dagger &= \hat{H} && (16)
\end{aligned}$$

Thus the time evolution of a quantum system is governed by the equation

$$i\hbar\frac{\partial}{\partial t}|\psi t\rangle = \hat{H}(t)|\psi t\rangle \tag{17}$$

Using correspondence with classical mechanics, Dirac shows that the operator $\hat{H}$ the represents the energy (or the Hamiltonian) of the system. (See §2 below and the discussion in the end of this section.) Using (3) in (18) we get

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)|\psi t_0\rangle = \hat{H}(t)U(t,t_0)|\psi t_0\rangle \tag{18}$$

This equation must hold for all vectors $|\psi >$. Hence the time evolution operator U must satisfy the differential equation

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = \hat{H}(t)U(t,t_0)\ . \tag{19}$$

§2 Time Development of Averages

Time variation of average values

The time evolution of a quantum system is governed by the Schrodinger equation

$$i\hbar\frac{d}{dt}|\psi t\rangle = \hat{H}|\psi t\rangle. \tag{20}$$

We will obtain an equation for time development of averages of a dynamical variable $\hat{F}$ The result will turn out to have an obvious correspondence with the classical equation of motion for dynamical variable F. This then will suggest the identification of $\hat{H}$ as the operator representing the Hamiltonian of the system.

Let $F(q,p,t)$ be an dynamical variable of the system and let $\hat{F}$ denote the corresponding operator. We are interested in finding out how the average value

$$\langle \hat{F} \rangle \equiv \langle \psi t|\hat{F}|\psi t\rangle \tag{21}$$

changes with time. The time dependence of the average value comes from dependence of the three objects, the operator$\hat{F}$, the bra vector $\langle \psi t|$, and the ket vector $|\psi t\rangle$, present in Eq.(21). The equation conjugate to the Schrodinger equation

$$i\hbar \frac{d}{dt}\,|\psi t\rangle = \hat{H}|\psi t\rangle \tag{22}$$

is given by

$$-\,i\hbar \frac{d}{dt}\,\langle \psi t| = \langle \psi t|\hat{H}^\dagger \tag{23}$$

Since the operator $\hat{H}$ is hermitian, the above equation takes the form

$$-\,i\hbar \frac{d}{dt}\,\langle \psi t| = \langle \psi t|\hat{H} \tag{24}$$

Therefore

$$\frac{d}{dt}\langle \hat{F}\rangle = \left(\frac{d}{dt}\langle \psi t|\right)\hat{F}|\psi t\rangle + \langle \psi t|\frac{d\hat{F}}{dt}|\psi t\rangle + \langle \psi t|\hat{F}\left(\frac{d}{dt}|\psi t\rangle\right) \tag{25}$$

Using Eq.(23) and Eq.(24) in Eq.(25) we get

$$\frac{d}{dt}\langle \hat{F}\rangle = -\frac{1}{i\hbar}\langle \psi t|\hat{H}\hat{F}|\psi t\rangle + \langle \psi t|\frac{d\hat{F}}{dt}|\psi t\rangle + \frac{1}{i\hbar}\langle \psi t|\hat{F}\hat{H}|\psi t\rangle \tag{26}$$

The above equation is rearranged to give the final form

$$\frac{d}{dt}\,\langle \hat{F}\rangle = \langle \frac{\partial}{\partial t}\hat{F}\rangle + \frac{1}{i\hbar}\langle\,[\hat{F},\hat{H}]\,\rangle \tag{27}$$

This result is known as Ehrenfest theorem. Comparing the Eq.(27) with the equation of motion in classical mechanics for time evolution of dynamical variables

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \{F,H\}_{PB} \tag{28}$$

and remembering that the commutator divided by $i\hbar$ corresponds to the Poisson bracket in the limit $\hbar \to 0$, we see that $\hat{H}$ must be identified as the operator corresponding to the Hamiltonian H of the system.

§3 Solution of Dependent Schrödinger Equation.

A scheme to solve the time dependent Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle \tag{29}$$

is described. The solution will be presented in the form

$$|\psi t\rangle = U(t, t_0)|\psi t_0\rangle \tag{30}$$

For our present discussion, it will be assumed that the Hamiltonian $\hat{H}$ does not depend on time explicitly. Let the state vector of system at initial time $t = 0$ be denoted by $|\psi_0\rangle$.

Since $\hat{H}$ is always assumed to be hermitian, its eigenvectors form an orthonormal complete set and we can expand the state vector at time t, $|\psi t\rangle$, in terms of the eigenvectors. Denoting the normalized eigenvectors by $|E_n\rangle$, we write

$$|\psi t\rangle = \sum_n c_n(t)|E_n\rangle. \tag{31}$$

where the constants $c_n(t)$ are to be determined. Substituting (**??**) in (**??**) we get

$$i\hbar\frac{d}{dt}\sum_n c_n(t)|E_n\rangle = \hat{H}|\psi t\rangle \tag{32}$$

$$i\sum_n \hbar\frac{dc_n(t)}{dt}|E_n\rangle = \sum_n c_n(t)\hat{H}|E_n\rangle \tag{33}$$

Taking scalar product with $|E_m\rangle$ and using orthonormal property of the eigenvectors $|E_n\rangle$, we get

$$i\hbar\frac{dc_m(t)}{dt} = E_m c_m(t). \tag{34}$$

which is easily solved to give

$$c_m(t) = c_m(0)e^{-iE_m t/\hbar}. \tag{35}$$

Therefore, $|\psi t\rangle$,the solution of time dependent equation becomes

$$|\psi t\rangle = \sum_m c_m(0)e^{-iE_m t/\hbar}.|E_m\rangle. \tag{36}$$

The coefficients $c_m(0)$ are determined in terms of the state vector $|\psi_0\rangle$ at time $t = 0$ by setting time $t = 0$ in the above equation. This gives

$$|\psi_0\rangle = \sum_n c_n(0)|E_n\rangle. \tag{37}$$

The unknown coefficients $c_n(0)$ can now be computed; taking scalar product of Eq.(87), with $|E_m\rangle$ we get

$$c_m(0) = \langle E_m|\psi_0\rangle. \tag{38}$$

Thus Eq.(86) and (**??**) give the solution of the time dependent Schrödinger equation as

$$\boxed{|\psi t\rangle = \sum_n c_n(0)\exp(-i\hbar E_n t)|E_n\rangle}. \tag{39}$$

The right hand side of the above equation can be rewritten as

$$\sum_n c_n(0)\exp(-i\hbar E_n t)|E_n\rangle = \sum_n c_n(0)\exp(-i\hbar H t)|E_n\rangle \tag{40}$$

$$= \exp(-i\hbar H t).\sum_n c_n(0)|E_n\rangle \tag{41}$$

Therefore Eq.(89) takes the form

$$|\psi t\rangle = \exp(-iHt/\hbar)|\psi_0\rangle. \tag{42}$$

In general, if the state vector is know at time $t = t_0$, instead of time $t = 0$, the result Eq.(90) takes the form

$$|\psi t\rangle = \exp(-iH(t-t_0)/\hbar)\sum_n c_n(t_0)|E_n\rangle \tag{43}$$

$$= \exp(-iH(t-t_0)/\hbar)|\psi t_0\rangle. \tag{44}$$

The time evolution operator $U(t, t_0)$, of Eq.(96), is therefore given by

$$\boxed{U(t, t_0) = \exp(-iH(t-t_0)/\hbar)}. \tag{45}$$

§4 Stationary States and Constants of Motion

Stationary states

Let us consider time evolution of a system if it has a definite value of energy at an initial time t_0. The value of the energy then has to be one of the eigenvalues and the state vector will be the corresponding eigenvector. So $|\psi t_0\rangle = |E_m\rangle$, then at time t the system will be in the state given by

$$|\psi t\rangle = U(t, t_0)|E_m\rangle = \exp(-iE_m(t-t_0)/\hbar)|E_m\rangle. \tag{46}$$

It must be noted that the state vector at different times is equal to the initial state vector times a *numerical phase factor* $(\exp(-iE_m(t-t_0)/\hbar))$. Therefore, the vector at time t represents the same state at all times. Such states are called **stationary states** because the state does not change with time. Every eigenvector of energy is a possible stationary state of a system. In such a state the average value of a dynamical variable, $\hat{X}$, not having time explicitly, is independent of time even if $\hat{X}$ does not commute with Hamiltonian. In fact the probabilities of finding a value on a measurement of the dynamical variable are independent of time.

Constant of motion

Unless mentioned otherwise, we shall always assume that the Hamiltonian H of the system under discussion is independent of time.

If the dynamical variable F does not contain explicit time dependence, then we have $\frac{\partial F}{\partial t} = 0$. If such an operator $\hat{F}$ commutes with the Hamiltonian operator $\hat{H}$, we will have

$$\boxed{[\hat{F}, \hat{H}] = 0}. \tag{47}$$

Eq.(**??**) shows that

$$\frac{d}{dt}\langle\psi t|\hat{F}|\psi t\rangle = 0$$

Therefore in an arbitrary state, the average value of $\hat{F}$ does not change with time. Such a dynamical variable will be called a **constant of motion**.

§5 Summary

- Given the state of the system at a time t_0, the state vector at any other time is related to it by a unitary transformation $U(t, t_0)$.

$$|\psi t\rangle = U(t, t_0)\,|\psi t_0\rangle$$

- The equation of motion of quantum system is the Schrodinger equation

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

  where $\hat{H}$ is the Hamltonian operator of the system.

- The time evolution operator satisfies the equation

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

- If the Hamiltonian does not depend on time, the evolution operator is

$$U(t, t_0) = \exp[-i\hat{H}(t - t_0)/\hbar]$$

- The average value of a dynamical variable,$\hat{F}$, satisfies

$$\frac{d}{dt}\langle\hat{F}\rangle = \langle\frac{\partial\hat{F}}{\partial t}\rangle + \frac{1}{i\hbar}\langle\,[\hat{F},\hat{H}]\,\rangle$$

- A dynamical variable is a constant of motion if it commutes with the Hamiltonian.

- The energy eigenstates of a system are staionary; they do not change with time. The state vector of a stationary state at any time is equal to the initial state vector multiplied by a numerical phase factor.

- The average value of a *constant of motion* G is independent of time in every possible state of the system including *nonstationary states.*

- The avearge value of *every* dynamical variable is independent of time in *stationary* states.

§6 Time Evolution of Quantum Systems-II

The state vector at a given time specifies the state of the system at a given time and the state at any time is obtained by solving the Schrödinger equation.

$$i\hbar\frac{d|\psi\rangle}{dt} = H|\psi t\rangle. \tag{48}$$

where H is the Hamiltonian operator. The reason for identification of H, in the above equation, with Hamiltonian is best brought out in by means of correspondence with equations in classical mechanics.

From now on we will assume that the Hamiltonian H does not depend on time. In this case the state vector at time t is related to the state vector at initial time t_0 by

$$|\psi t\rangle = U(t,t_0)|\psi t_0\rangle \tag{49}$$

where

$$U(t,t_0) = \exp\Big(-\frac{iH(t-t_0)}{\hbar}\Big) \tag{50}$$

Since H is a hermitian operator, it follows that $U(t,t_0)$ is aunitary operator.

The Hamiltonian operator being Hermitian leads to the following important consequences. In the table below a few examples of time evolution of states are given.

Table : Time evolution energy eigenstates of a quantum system

S.N.	State at time $t = 0$	State at time t
1.	$\vert E_n\rangle$	$e^{-iE_nt/\hbar}\vert E_n\rangle$
2.	$c_1\vert E_n\rangle + c_2\vert E_n\rangle$	$c_1e^{-iE_nt/\hbar}\vert E_1\rangle + c_2e^{-iE_2t/\hbar}\vert E_n\rangle$
3.	$\sum_k c_k\vert E_k\rangle$	$\sum_k c_ke^{-iE_kt/\hbar}\vert E_k\rangle$
4.	If states $\vert\psi t_0\rangle, \vert\phi t_0\rangle$ then $c_1\vert\psi t_0\rangle + c_2\vert\phi t_0\rangle$	evolve into $\vert\psi t\rangle, \vert\phi t\rangle$, evolves into $c_1\vert\psi t\rangle + c_2\vert\phi t\rangle$

- The first row in the table shows that the energy eigenstates

$$H|E_n\rangle = E_n|E_n\rangle \tag{51}$$

i.e. the states corresponding to a definite value of energy, have a very simple time evolution. The state vector changes by phase factor, a multiplicative constant of absolute value 1. Thus the state itself does not change with time. Therefore energy states are called *stationary states.*

- The time evolution preserves the superposition of states as is brought out by the examples in the second and last rows of the table.

- The time evolution is unitary and hence norm of the state vector is preserved. Mathematically this means that the norm $\langle\psi t|\psi t\rangle$ is independent of time. In other words

$$\langle\psi t|\phi t\rangle = \langle\psi t_0|\phi t_0\rangle \tag{52}$$

$$\text{and} \quad \frac{d\|\psi(t)\|}{dt} = 0 \tag{53}$$

Remembering that $\|\psi(t)\|^2$ is just the sum of probabilities of all possible outcomes, The above result has a physical interpretation total probability of all possible outcomes of a measurement remains constant $(= 1)$ at all times.

Here the results given above are a consequence of Hamiltonian being hermitian.

In an alternate approach [**?**], one can start from requirements that superposition be preserved and the normalization of the state vector should not change with time and prove that this leads to an equation of the form

(??) where H some hermitian operator. Identification with operator corresponding to Hamiltonian can then be done by making use of classical correspondence.

§7 Heisenberg Picture of Quantum Mechanics

§7.1 A Summary of Schrodinger Picture

In most commonly used description of quantum mechanics, the time development is described by the time dependent Schrödinger equation.

$$i\hbar\frac{\partial|\psi t\rangle}{\partial t} = H|\psi t\rangle \tag{54}$$

where H is the Hamiltonian operator of the system. The dynamical variables are operators and do not evolve with time. This description of time evolution is known as the *Schrodinger picture* of quantum mechanics.

Note that average values and probabilities are observable quantities, but not the wave function or the state vector. This fact allows to describe the time development in several possible ways. We will describe two alternate important ways of describing time development of a quantum system known as the Heisenberg picture and the Dirac picture.

We use subscript S to denote the Schrodinger picture states $|\psi\rangle_S$ and operators $X_S(q,p)$ or simply X_S.

To simplify present discussion, we will assume that the Hamiltonian is independent of time. The state vector at time t is given by

$$|\psi t\rangle_S = U(t,t_0)|\psi_{t_0}\rangle_S \tag{55}$$

where the time evolution operator is given by

$$U(t,t_0) = \exp(-iH(t-t_0)/\hbar). \tag{56}$$

Without loss of generality, we will set $t_0 = 0.$ and write

$$|\psi t\rangle_S = e^{-iHt/\hbar}|\psi_0\rangle \tag{57}$$

§7.2 Heisenberg Picture

The Heisenberg picture state vector is defined by

$$|\psi t\rangle_H = e^{iHt/\hbar}|\psi t\rangle_S = |\psi_0\rangle. \tag{58}$$

The Heisenberg state vector is independent of time and coincide with the state vector in the Schrödinger picture at initial time. The time development of the Heisenberg picture operators is defined so that the average value of any dynamical variable at time t in the Schródinger and Heisenberg pictures coincide. Thus we demand

$$ {}_H\langle\psi t|X_H(t)|\psi t\rangle_H = {}_S\langle\psi t|X_S|\psi t\rangle_S \tag{59}$$

Substituting (84) and (85) gives

$$\langle\psi_0|X_H(t)|\psi_0\rangle = \langle\psi_0|e^{iHt/\hbar}\, X_S\, e^{-iHt/\hbar}|\psi_0\rangle. \tag{60}$$

We, therefore, define the Heisenberg picture operators by

$$X_H(t) = e^{iHt/\hbar}\, X_S\, e^{-iHt/\hbar}. \tag{61}$$

Equation of Motion In Heisenberg picture the state vector does not evolve with time. SO how do we describe the time development of a system? The answers is that in the Heisenberg picture the operators carry the entire time dependence. So for a point particle, the position operator, the momentum operator, in fact all dynamical variables become time dependent. This is parallel to the classical description the time evolution of the state is described by the position and momentum. The equations of motion are then the equations telling us how the a given dynamical variable will change with time. The equation of motion is easily derived from Eq.(88) and we compute

$$\frac{dX_H}{dt} = \frac{d}{dt}\Big[e^{iHt/\hbar}\, X_S\, e^{-iHt/\hbar}\Big] \tag{62}$$

$$= \frac{d}{dt}\Big(e^{iHt/\hbar}\Big)\, X_S\, e^{-iHt/\hbar} + e^{iHt/\hbar}\left(\frac{d}{dt}X_S\right) e^{-iHt/\hbar} + e^{iHt/\hbar}\, X_S\, \frac{d}{dt}\Big(e^{-iHt/\hbar}\Big) \tag{63}$$

$$= \tfrac{iH}{\hbar}e^{iHt/\hbar}\, X_S\, e^{-iHt/\hbar} + e^{iHt/\hbar}\left(\frac{\partial}{\partial t}X_S\right) e^{-iHt/\hbar} + e^{iHt/\hbar}\, X_S\, e^{-iHt/\hbar}\tfrac{-iH}{\hbar} \tag{64}$$

$$= \frac{i}{\hbar}HX_H + \frac{\partial}{\partial t}X_H - X_H\frac{i}{\hbar}H \tag{65}$$

Here we have used

$$\frac{d}{dt}e^{iHt/\hbar} = (\tfrac{iH}{\hbar})e^{iHt/\hbar} = e^{iHt/\hbar}(\tfrac{iH}{\hbar}). \tag{66}$$

Thus we arrive at the final form of equations of motion in the Heisenberg picture

$$\boxed{\frac{dX_H}{dt} = \frac{\partial X_H}{\partial t} + \frac{1}{i\hbar}\big[X_H, H\big]_-.} \tag{67}$$

Recalling that the ($\frac{1}{i\hbar}\times$ commutator) has correspondence with the Poisson bracket, we have an obvious correspondence with the Poisson bracket form of equations of motion in classical mechanics.

The steps (89)- Eq.(92), leading to the final result (93), require some explanation and care as explained in Notes and Comments section at the end.

§8 Interaction Picture of Quantum Mechanics

We shall now discuss the interaction picture, also known as Dirac picture. We shall denoting the Schrodinger picture kets and operators by $|\psi\rangle_S, X_S$ etc. and $|\psi\rangle_I, X_I$ etc will denote the corresponding quantities in the interaction picture.

Let the Hamiltonian of the system be written as sum of two parts

$$H = H_0 + H'. \tag{68}$$

H_0, H' will be called free part and the interaction part of the Hamiltonian H, respectively. While H_0 is assumed to be independent of time, the interaction Hamiltonian may or may not depend on time. The state of a system in the interaction picture are defined by

$$|\psi t\rangle_I = e^{iH_0t/\hbar}|\psi t\rangle_S. \tag{69}$$

and the dynamical variables of the interaction picture are defined by demanding that the average values in the interaction and Schrödinger pictures coincide at all times:

$$_I\langle\psi|X_I|\psi\rangle_I \equiv_S \langle\psi|X_I|\psi\rangle_S. \tag{70}$$

Substituting

$$|\psi t\rangle_S = e^{-iH_0t/\hbar}|\psi t\rangle_I, \tag{71}$$

from (83) we get

$$_I\langle\psi|X_I|\psi\rangle_I = {_I\langle\psi|}e^{iH_0t/\hbar}X_I e^{-iH_0t/\hbar}|\psi\rangle_I. \tag{72}$$

Therefore, we use

$$X_I = e^{iH_0t/\hbar}X_S e^{-iH_0t/\hbar} \tag{73}$$

to define the an interaction picture dynamical variables.

The time dependence of the interaction picture operators is very simple and is governed by the free Hamiltonian H_0:

$$i\hbar\frac{dX_I(t)}{dt} = \big[X_I, H_0\big]. \tag{74}$$

As an example, it should be obvious that, the free particle Hamiltonian H_0 in the interaction picture remains identical with H_0:

$$(H_0)_I = e^{iH_0t/\hbar}H_0 e^{-iH_0t/\hbar} = H_0. \tag{75}$$

On the other hand, even though the interaction part of the Hamiltonian, H', may be independent of time, the interaction picture Hamiltoinan H'_I

$$H'_I(t) = e^{iH_0t/\hbar}H' e^{-iH_0t/\hbar} \tag{76}$$

is different from H' and depends explicitly on time. The time dependence of the state vector in the interaction picture is governed by this operator H'_I, the interaction part of Hamiltonian,H', transformed to the interaction picture. We will now derive the differential equation which gives the evolution of the state vectors. For this purpose we begin with (83)

$$\begin{aligned}
i\hbar\frac{d}{dt}|\psi t\rangle_I &= i\hbar\frac{d}{dt}\Big(e^{iH_0t/\hbar}|\psi t\rangle_S\Big) \\
&= i\hbar\Big(\frac{d}{dt}e^{iH_0t/\hbar}\Big)|\psi t\rangle_S + e^{iH_0t/\hbar}\Big(i\hbar\frac{d}{dt}|\psi t\rangle_S\Big) + \qquad (77) \\
&= -H_0 e^{iH_0t/\hbar}|\psi_0\rangle_S + e^{iH_0t/\hbar}\big(H_0 + H'\big)|\psi t\rangle_S \\
&= e^{iH_0t/\hbar}(-H_0)|\psi_0\rangle_S + e^{iH_0t/\hbar}\big(H_0 + H'\big)|\psi t\rangle_S \\
&= e^{iH_0t/\hbar}\big(H'\big)|\psi t\rangle_S \qquad (78)
\end{aligned}$$

Next, we need to express the Schrödinger picture state vector,$|psit\rangle_S$, in the right hand side in terms of the interaction picture state vector $|\psi t\rangle_I$. Thus we get

$$i\hbar\frac{d}{dt}|\psi t\rangle_I = e^{iH_0t/\hbar}\big(H'\big)e^{-iH_0t/\hbar}|\psi t\rangle_I. \qquad (79)$$

Thus we get the desired equation for time evolution of the state vectors in the interaction picture in the final form

$$\boxed{i\hbar\frac{d}{dt}|\psi t\rangle_I = H'_I|\psi t\rangle_I} \qquad (80)$$

where H'_I is given by Eq.(90). The state vector evolves with the interaction part of the Hamiltonian.

§9 Perturbation Expansion in Interaction Picture

§9.1 Integral equation for time evolution operator

Let $H = H_0 + H'$ be the Hamiltonian of system of interest, H_0 and H', respectively, being the free part and interacting part of the total Hamiltonian . In the interaction picture the time dependence of an operator is given by

$$i\hbar\frac{dX_I(t)}{dt} = [X_I(t), H_0]. \qquad (81)$$

The solution of this equation can be written down explicitly and we have

$$X_I(t) = e^{iH_0t/\hbar}X_I(0)e^{-iH_0t/\hbar}. \qquad (82)$$

The time development of the state vector in the interaction picture is given by the Schrodinger equation

$$i\hbar|\psi t\rangle_I = H'_I(t)|\psi t\rangle. \tag{83}$$

It must be noted that the interaction Hamiltonian in the interaction picture, $H'_I(t)$, is always time dependent whether the Schrodinger picture operator depends on time or not. This makes it impossible to write an explicit solution to (83) impossible. Here we will be interested in deriving a perturbative expansion in powers of $H'_I(t)$.

Let $U(t,t_0)$ be unitary operator which connects the interaction picture states at times t, t_0):

$$|\psi t\rangle_I. = U(t,t_0)|\psi t_0\rangle_I. \tag{84}$$

Obviously we must have

$$U(t_0,t_0) = \hat{I}. \tag{85}$$

Substituting (84) in both sides of Eq.(83), we get the following equation for the time evolution operator $U(t,t_0)$.

$$i\hbar\frac{d}{dt}U(t,t_0)|\psi t_0\rangle_I = H'_I(t)U(t,t_0)|\psi t_0\rangle_I. \tag{86}$$

Since the initial state $|\psi, t_0\rangle$ is arbitrary, we get

$$\boxed{i\hbar\frac{d}{dt}U(t,t_0) = H'_I(t)U(t,t_0).} \tag{87}$$

Integrating this equation w.r.t. time and using the initial condition (85) we get

$$\boxed{U(t,t_0) = \hat{I} + \frac{1}{i\hbar}\int_{t_0}^{t} H'(t)U(t,t_0)\,dt.} \tag{88}$$

This integral equation is starting point for a perturbative expansion of the time evolution operator $U(t,t_0)$.

§9.2 Perturbative solution

In order to simplify the notation, we will drop the suffix I from $H'_I(t)$ and use the notation $H'(t)$ to denote the interaction picture operator.

For book keeping purpose we rewrite equation (88) as

$$U(t,t_0) = \hat{I} + \frac{\lambda}{i\hbar}\int_{t_0}^{t} H'(t)U(t,t_0)\,dt \tag{89}$$

and the parameter λ will be set equal to unity in the end. As zeroth order approximation we may write

$$U^{(0)}(t,t_0) = \hat{I} \tag{90}$$

and obtain the next approximation by inserting the above expression in the right hand side of (89). This gives

$$U^{(1)}(t,t_0) = \hat{I} + \frac{\lambda}{i\hbar}\int_{t_0}^{t} H'(t_1)\,dt_1. \tag{91}$$

Repeating this process, by inserting $U^{(1)}(t,t_0)$ for $U(t,t_0)$ in the right hand side of Eq.(89), we get the second order approximation as

$$U^{(2)}(t,t_0) = \hat{I} + \frac{\lambda}{i\hbar}\int_{t_0}^{t_1} H'(t)dt_1 + \Big(\frac{\lambda}{i\hbar}\Big)^2 \int_{t_0}^{t}\int_{t_0}^{t_1} H'(t_1)H'(t_2)\,dt_2dt_1. \tag{92}$$

Iterating the above process gives an infinite series in powers of λ, The double integral in the right hand side can be written as

$$\int_{t_0}^{t}\int_{t_0}^{t_1} H'(t_1)H'(t_2)\,dt_2dt_1 = \frac{1}{2}\int_{t_0}^{t}\int_{t_0}^{t} T\big(H'(t_1)H'(t_2)\big)\,dt_2dt_1. \tag{93}$$

Here the symbol T stands for time ordering, defined by,

$$T\big(H'(t_1)H'(t_2)\big) = \begin{cases} H(t_1)H(t_2), & \text{if} \quad t_1 > t_2, \\ H(t_2)H(t_1), & \text{if} \quad t_2 > t_1. \end{cases} \tag{94}$$

Proof of Eq.(93) is left as an exercise in double integration.

Later terms of the series can be found and turn out to be multiple integral of time ordered product of more factors of $H'(t)$:

$$U(t,t_0) = I + \sum_{n=1}^{\infty}\Big(\frac{1}{i\hbar}\Big)^n \int_{t_0}^{t} dt_1 \ldots \int_{t_0}^{t} dt_n T\big\{H(t_1)H(t_2)\ldots H(t_n)\big\}. \tag{95}$$

Retaining first few terms in the above series gives useful approximation for several applications. The series (95) is symbolically written as

$$U(t,t_0) = T\exp\left(\frac{-i}{\hbar}\int_{t_0}^{t} H(t)dt\right). \tag{96}$$

and the right hand side is known as *time ordered exponential* of the argument.

References

[1] See QuestionBank file `qm-que-03001.pdf`