

# **FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH**

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## **Open Quantum Systems: Introduction - Part 01**

Everything around us is made of atoms and molecules and atoms and molecules satisfy quantum mechanical laws. Therefore, everything should satisfy on a fundamental level, the quantum mechanical laws, but still we do not see the superposition entanglement and measurement collapse in our daily life. Where is the discrepancy? Where does we stop seeing the quantum effects and classical effects start dominating? That is one fundamental and profound questions which we will try to answer in the following topic. Our next topic of discussion is open quantum system.

This is an attempt to understand the lack of quantumness on a macroscopic level, emergence of classicality, lack of quantumness or coherence and stuff like that. Open quantum system treatment also help us answer the question of spontaneous emission and the noise in quantum information theory. So, we will start this discussion with classifying the type of quantum system. So, there are three major type of quantum system. One is the isolated quantum system.

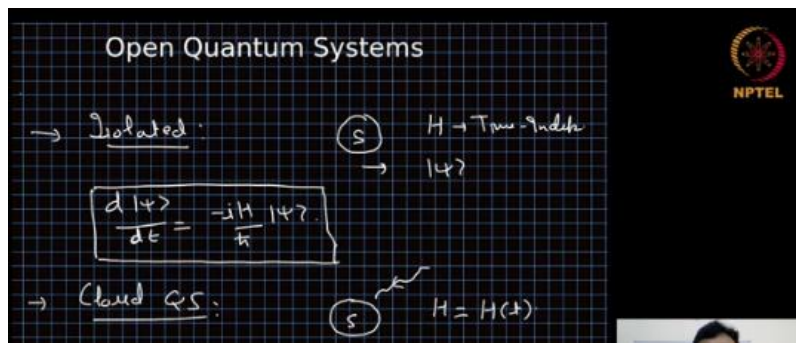
An isolated quantum system is a quantum system which is not interacting or coupled with any other surrounding system. We have a quantum system, does not matter how big or small it is, but this system is not interacting with anything else. The signature of this system is the Hamiltonian is time independent. And the state of the system is always pure. An isolated quantum system should be or will be in a pure state forever.

And the Schrodinger equation is the defining equation for the dynamics. And these are very ideal quantum systems. Whenever we start our first lecture in any quantum mechanical course, the quantum system under consideration is typically an isolated quantum. This is the simplest system to explain and to do calculations, but it is not physical unless we consider the entire universe as a single quantum system. If there is an isolated quantum system and by definition it is not interacting with anything else, it

means we cannot observe it. As an observer, we cannot observe it, we cannot find out the presence of this. So, in that way isolated quantum systems are hypothetical we can say, in that way isolated quantum systems are good for understanding the quantum mechanics but may not be very physical.

That brings us to the next level of quantum system, next type of quantum system and that is closed quantum system. They are the system which the quantum system has and it is interacting with some system which can be treated classically. For example, an atom interacting with electromagnetic light. If we consider the electromagnetic field as a classical field, then the whole, the system, the atom can be treated as quantum mechanically. And this is one example of a closed quantum system.

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The typical signature of this quantum system is Hamiltonian is time dependent. So, Hamiltonian is a function of time. So, there the closed quantum system can be in pure state as well as in the mixed state. The dynamical equation of a closed quantum system can be written as  $\rho \dot{=} -i$  over  $\hbar$  commutator of  $H$  with  $\rho$  or we can say some, some map acting on  $\rho$  at time  $t$  and this  $L$  is a super operator or quantum map and let us say  $L$  is the matrix representation of it of the map  $L$ , so we get the equation  $\rho \dot{=} L \rho$  where  $\rho$  is the vector vectorized form of  $\rho$  this is the unfolded vector of  $\rho$ . So, let me remind you if the  $\rho$  is a  $2 \times 2$  matrix with elements  $a, b, c, d$ , then the vector  $\rho$  will be  $a, b, c, d$ . And this ordering is very important.

It cannot be  $a, c, b, d$ . If it is  $a, c, b, d$ , then we have to change the  $L$  matrix also and few other things will change. So, we are sticking with the convention that it is  $a, b, c, d$ . So, in that way the dynamical equation can be written as the time derivative of a  $\rho$  vector is equal to the matrix  $L$ , which is the matrix representation of the map  $L$  here acting on  $\rho$ . From here, we can write a general solution or formal solution for the state  $\rho$  or  $\rho$  vector as exponential of  $L t$  acting on  $\rho$  if  $L$  is time independent that is the case of

isolated system and exponential of 0 to t L ds acting on rho where this operator is the time ordering operator acting on rho. It is a little bit complicated expression, but it is the solution for a state of a system when that Hamiltonian is time dependent.

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$$\dot{\rho} = -\frac{i}{\hbar} [H(t), \rho]$$

$$= \mathcal{L}[\rho]$$

$$\boxed{|\rho\rangle = L|\rho\rangle}$$

$$\rho = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \rightarrow |\rho\rangle = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

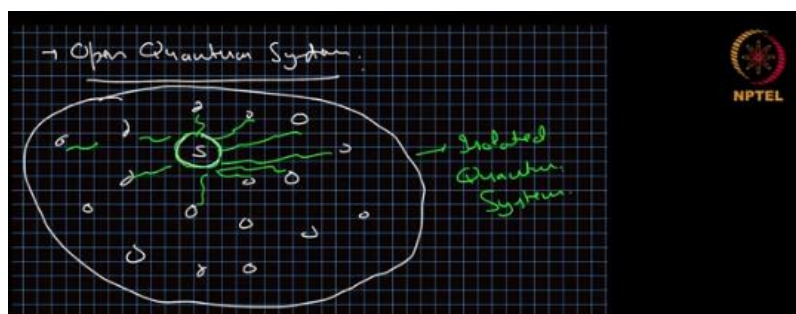
$$|\rho_t\rangle = \exp\left[-\frac{i}{\hbar} \int_0^t L ds\right] |\rho_0\rangle \text{ if } L \text{ time-independent}$$

$\mathcal{L} \rightarrow$  Superoperator  $\rightarrow$  Map.  
 $L \leftrightarrow \mathcal{L}$

$|\rho\rangle \rightarrow$  vectorized form of  $\rho$ .

This is the initial state rho zero and here the state is rho zero. The third type of quantum system which we are interested in are the open quantum. Open quantum systems are quantum systems as which are interacting with many of other quantum systems, so they are in a bath of lot of quantum systems there is interaction between all these systems with different varying interactions. And the whole quantum system can be treated as one isolated quantum system. So, open quantum system is a subsystem, a very small subsystem of a very very large quantum system large isolated quantum system and we are interested in only in the dynamics of a very small part. So, in this case our total Hilbert space H is the Hilbert space of the system under consideration or the system of interest can serve the system of the surrounding we can call it environment or we can call it bath or we can call it reservoir.

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So, we will be using these words interchangeably. So, sometimes we will call it environment or bath or reservoir. So, our total system which is total Hilbert space  $H$  will be a tensor product of the system Hilbert space and the environment Hilbert space. Our state will also be the state of system and bath. And since the whole system is isolated, but we will generally treat it as a mixed state in the beginning.

So, the dynamics will be given by  $U_{SB}$ . Dynamics of this will be given by a unitary matrix  $U_{SB}$  which will be exponential of minus  $i H_{SB} t$  over  $\hbar$  where  $H_{SB}$  is the Hamiltonian of the system and bath together. Typically, the Hamiltonian  $H_{SB}$  will be the free Hamiltonian of the system plus free Hamiltonian of the bath plus the interaction between system and bath. In general, we will consider this interaction between system and bath as time dependent. But typically, since we are assuming the total system and bath to be isolated system, so even all three Hamiltonians here will be time independent in general.

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$$H = H_S \otimes I_E$$

$$\rho = \rho_{SB}$$

$$\rightarrow U_{SB} = \exp\left[-j \frac{H_{SB} t}{\hbar}\right]$$

$E \rightarrow$  Environment  
 $B \rightarrow$  Bath  
 $R \rightarrow$  Reservoir

This actually is  $H_S$  tensor identity for bath plus identity for system plus tensor Hamiltonian of bath plus the Hamiltonian acting on both system and bath. So, the time evolution of the total system and bath is  $U_{SB}(t, t_0) \rho$  at zero let me  $U_{SB}$ , this is  $U_{SB}$ ,  $U_{SB}^\dagger U_{SB}(t, t_0)$ , this is the total evolution of the system and bath together and then from here we can calculate  $\rho_S$  at time  $t$  that is trace over bath  $\rho_{SB}$  at time  $t$  equals trace over bath  $U_{SB}(t, t_0) \rho_{SB}$  at 0 and  $U_{SB}^\dagger$  at  $t$ . The same equation, I'm just writing it again here. I don't want to write again as  $B$  and  $t_0$  all those things. If that is  $t_0$ , then it should also be  $t_0$  here.

This also should be  $t_0$ . So, this is how we can get the dynamics of a system when it is interacting with other systems and with environment. So, we can understand the whole

dynamics from this flowchart. We have system. We have the state of the system and bath together at time 0.

This belongs to the operators acting on HS tensor HB. And then we do the unitary evolution,  $U_{SB}$ , and we get  $\rho_{SB}$  at time t. And then we trace out the bath and we get  $\rho_S$  of time t. There is other way that we trace out the bath in the beginning and we get  $\rho_S$  at time 0. And from here, we can do the open system dynamics. So, we have two ways of arriving at the time evolved state of the system. One, by considering the full treatment where we have system and bath in some initial state.

We have a unitary evolution of the system and bath and we get the final state of system and bath. From there, we can trace out the bath state of freedom. Other is, we can trace out the bath degree of freedom in the beginning itself, so that we have only the state of the system and then we perform our open system dynamics. Now what is this open system dynamics is here to be figured out, but what are the advantages of this second approach and what are the advantages of the first approach, first approach and second approach? So, we have two approaches to solve the dynamics of a system interacting with bath. One is where we consider the initial state of the system and bath together.

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$$\rho_{SB}(t) = U_{SB}(t, t_0) \rho_{SB}(t_0) U_{SB}^\dagger(t, t_0)$$

$$\rightarrow \rho_S(t) = \text{Tr}_B(\rho_{SB}(t)) = \text{Tr}_B[U(t) \rho_{SB}(t_0) U^\dagger(t)]$$

The flowchart shows two paths:
 

- Path I:**  $\rho_{SB}(0) \in \mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_B) \xrightarrow{U_{SB}} \rho_{SB}(t) \xrightarrow{\text{Tr}_B} \rho_S(t)$
- Path II:**  $\rho_{SB}(0) \xrightarrow{\text{Tr}_B} \rho_S(0) \xrightarrow{\text{Open System Dynamics}} \rho_S(t)$

Assuming system and bath is a isolated system, then the initial state will be generally a pure state. Then we do the unitary dynamics which can be solved using the Schrodinger equation and then we trace out the bath degree of freedom to get the final state of the system. In this approach we are using the familiar techniques where we use the Schrodinger equation, we calculate the unitary evolution from the Hamiltonian of the system and bath and then we get the final state of the system. But in this approach, there

is a problem that it requires the full knowledge of the Hamiltonian of the system and bath and it assumes that we can solve such large system if the bath is very very large. On the other hand the second approach where we trace out the bath degree of freedom in the beginning itself and we get the initial state of the system and then we perform a modified dynamics of the system of position dynamics to arrive at the final state.

In this approach, we need to work only with the system state and we don't need the full information about the Bath Hamiltonian. What we need is the correlation functions of the interaction Hamiltonian from the Bath Hamiltonian. That will get clear soon when we derive the dynamical equation for open quantum system dynamics and we will know that why this technique is more powerful. So, we start with the Hamiltonian of the system and bath that is HS, that is HS tensor identity. It is the free-Hamiltonian of the system.

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$$H = \underbrace{H_S}_{\text{Free Hamiltonian System}} + H_B + H_I$$

$$i \frac{d\rho}{dt} = [H, \rho] \quad \rho \in \mathcal{S}(H_S \otimes H_B)$$

$$i \text{Tr}_B \left( \frac{d\rho}{dt} \right) = \text{Tr}_B [H, \rho]$$

$$\Rightarrow i \frac{d\rho_S}{dt} = \text{Tr}_B [H, \rho]$$

What we mean by free-Hamiltonian? This is the Hamiltonian of the system when the bath is not present plus HB, that is the free Hamiltonian of the bath plus HI, that is the interaction Hamiltonian between system and bath. Then we can write d rho over dt, i over h bar, for the sake of simplicity we will just use h bar to be 1, so it's i d rho over dt will be the commutator of H with rho where rho is the state of the system and bath together Then we can trace our bath in this dynamical equation we get i rho s over d rho s over dt equals trace over bath with the commutator of H and rho. So, this is our simplified dynamical equation where H is the total Hamiltonian of the system and bath, rho is the total state of system and bath and rho s is the reduced density matrix of the system at time t.

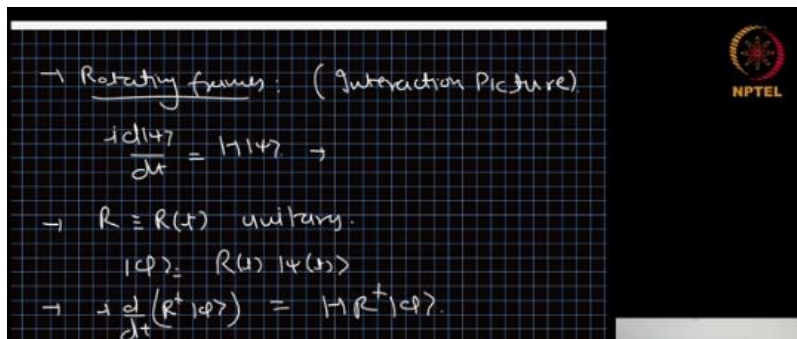


So, the Hamiltonian  $H$  has many terms, one is the free Hamiltonian of the system, free Hamiltonian of the bath and the interaction Hamiltonian. To reduce the difficulty and to make the calculation simple, it is often beneficial to work in rotating frames. This is also known as an interaction picture. In rotating frame, let us say we have a Hamiltonian  $H$  and we want to find the dynamics of the system. So, we have  $i \frac{d\psi}{dt} = H \psi$ .

Now, let us define a unitary  $R$  which is a time dependent unitary and then we define the state  $\phi$  which is  $R$  acting on  $\psi$ . So,  $\phi$  is a time dependent, time dependent state, which is, which can be achieved by applying the unit, time dependent unitary  $R$  on the time dependent state  $\psi$ . Let me write explicitly time here. As we know, unitary transformations are rotations in the Hilbert space. So, in that way,  $\phi$  is a continuously rotating state  $\psi$ .

Now, if we want to find the same dynamical equation in terms of  $\phi$ , how will it go? That we can write  $i \frac{d\psi}{dt}$ ,  $\psi$  can be written as  $R^\dagger \phi$ , that is  $H R^\dagger \phi$ . So, the same equation, the dynamical Schrodinger equation can be written in terms of  $\phi$  as this, which is equal to  $i \frac{dR^\dagger}{dt} \phi + R^\dagger \frac{d\phi}{dt}$ . That is  $H R^\dagger \phi$ . If you multiply the whole equation by  $R$  from the left, then we get  $i R \frac{dR^\dagger}{dt} \phi + \frac{d\phi}{dt} = R H R^\dagger \phi$  acting on  $\phi$  or we can write it as  $i \frac{d\phi}{dt} = R H R^\dagger \phi - i R \frac{dR^\dagger}{dt} \phi$ .

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From here, we can say that the dynamical equation for the state  $\phi$  which is the rotated version of the state  $\psi$  is  $i \frac{d\phi}{dt} = H_{\text{effective}} \phi$ , where  $H_{\text{effective}}$  is nothing but  $R H R^\dagger - i R \frac{dR^\dagger}{dt}$ . So, the dynamics of the rotating state can be defined by an effective Hamiltonian  $H_{\text{effective}}$  which can be written in terms of the original Hamiltonian  $H$  and the rotation matrix  $R$ . So, sometime this representation can make our life simpler. For example, in the case where total Hamiltonian is  $H_0 + H_1$ , where we have just divided the Hamiltonian into two parts,

$H_0$  and  $H_1$  part. For some reasons, we will see what are the implications of that. And  $R$  is defined as exponential of  $i H_0 t$ . Then first of all, we can see that  $dR$  dagger over  $dt$  is minus  $i H_0$  times exponential of  $i H_0 t$  which is minus  $i H_0 R$  dagger  $R$  dagger or minus  $i R dR$  dagger over  $dt$  is minus  $R H_0 R$  dagger.

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$$\begin{aligned} &\rightarrow i \left( R \frac{d\phi}{dt} + \frac{dR}{dt} \phi \right) = R H R^\dagger |\phi\rangle \\ &= i \frac{d\phi}{dt} = \left( R H R^\dagger - i R \frac{dR^\dagger}{dt} \right) |\phi\rangle \\ &= i \frac{d\phi}{dt} = H_{\text{eff}} |\phi\rangle \\ &H_{\text{eff}} = R H R^\dagger - i R \frac{dR^\dagger}{dt} \\ &H = H_0 + H_1 \end{aligned}$$

But  $R$  is a function of  $H_0$ , so  $R$  and  $R$  dagger commute, so it becomes minus  $H_0$ . Further,  $R H R$  dagger, that is the first term in the effective Hamiltonian,  $R H R$  dagger, that will become  $R H_0$  plus  $H_1 R$  dagger. That will be  $H_0$  because  $R$  commutes with  $H_0$ , so it will just give you  $R H_0 R$  dagger will be just  $H_0$  plus  $R H_1 R$  dagger. With these two expressions, we can find the effective Hamiltonian to be  $H_0$  plus  $R H_1 R$  dagger minus  $H_0$  that will be  $R H_1 R$  dagger. So, in that way, the effective Hamiltonian does not have both  $H_0$  and  $H_1$  directly but a new term which is  $R H_1 R$  dagger, so sometimes this formalism can yield a very simple effective Hamiltonian to find the dynamics. So, from the effective Hamiltonian, we can find the dynamics of the rotating state  $\phi$  and from there we can find the dynamics for  $\psi$ . So, if we make a flow chart it will be  $H$ , which is  $H_0$  plus  $H_1$  goes to  $H$  effective which yields the dynamics of the rotating frame, rotating state  $\phi$  which in turn yields the dynamics of the state  $\psi$ , so we could have done it from  $H$  to  $\psi$ .

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$$\begin{aligned} \frac{dR^\dagger}{dt} &= -i H_0 R^\dagger \\ \rightarrow -i R \frac{dR^\dagger}{dt} &= -R H_0 R^\dagger = -H_0 \\ R H R^\dagger &= R (H_0 + H_1) R^\dagger = H_0 + R H_1 R^\dagger \\ H_{\text{eff}} &= H_0 + R H_1 R^\dagger - H_0 = R H_1 R^\dagger \end{aligned}$$



But sometimes it's difficult to work with this thing because of the complicated form of the Hamiltonian. But and when we go to the rotating frame, this H effective is the Hamiltonian in the rotating frame, which is equivalent to the H in the stationary frame. And the state phi is the state in the rotating frame corresponding to the state psi in the stationary frame. So, we go from H to H effective and in this process, we define a rotation matrix R which is a time dependent rotation and the same transformation we have to apply on phi on psi to get phi and we can find the dynamics. We will be using this formalism quite a bit when we are dealing with open quantum system dynamics.

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$$RHR^\dagger = R[H_0 + H_I]R^\dagger = H_0 + R H_I R^\dagger$$

$$H_{eff} = H_0 + R H_I R^\dagger - H_0 = R H_I R^\dagger$$

$$H = H_0 + H_I \rightarrow H_{eff} \rightarrow |\varphi(t)\rangle \rightarrow |\psi(t)\rangle$$

$$\psi \rightarrow |\psi(0)\rangle$$

Now we go back to the open quantum system where our total Hamiltonian is HS plus HB plus H interaction. Let us call this as H0 and this becomes H1, HI we just keep it as H. So, the effective Hamiltonian will be HI of t which will be R HI R dagger and R will be exponential of i HS plus HB t let me remind you that we have this is hs plus hb times t not over h bar because we have assumed h bar to be 1. So, we saw that state psi goes to phi, which is R acting on psi. Similarly, state rho will go to rho interaction picture we can write as R rho R dagger.

And then we can write the dynamical equation for the state rho, rho I dot will be minus i H effective times rho I. H effective we write or HI, which is a function of time. So, we have to solve now this dynamical equation to in order to get the dynamics of the system and the bath and the total dynamics. And from here, if we trace our bath, we get the system interaction Hamiltonian or density matrix at time t, we just total, that is actually rho SI dot t and that will be trace over bath minus i HI rho.

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$$H = H_S + H_B + H_I$$

$$H_0 = H_S + H_B$$

$$H_{eff} = H_I(t) = R H_I R^\dagger$$

$$R = e^{i(H_S + H_B)t}$$

$$|\psi\rangle \rightarrow |\varphi\rangle = R|\psi\rangle$$

$$\rho \rightarrow \rho_I = R\rho R^\dagger$$

$$\dot{\rho}_I = -i[H_I(t), \rho_I]$$

