

# FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

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Week-10  
Lecture-29

## Open Quantum Systems: Introduction - Part 02

So, formally this equation  $\dot{\rho}_I - i H_I \rho_I$  can be solved as follows.  $\rho_I$  at time  $t$  will be  $\rho_I$  at 0 minus  $i$  integration  $H_I \rho_I$  from 0 to  $t$ . So here we have solved for  $\rho_I$  in terms of  $\rho_I$ , so it's a recursive solution and we can substitute  $\rho_I$  in this expression to get the second order so  $\rho_I$  becomes  $\rho_I$ ,  $\dot{\rho}_I$  again becomes  $-i H_I \rho_I$  minus  $i$  0 to  $t$   $H_I \rho_I$   $H_I \rho_I$   $ds$ . This is the recursive solution of the dynamical equation in terms of  $\rho_I$ . Let us drop the subscript  $I$  from here on. Every state and Hamiltonian is in interaction picture. So, we don't need to write subscript  $I$  which represents the interaction picture.

And this will make the expression a little bit simpler. Let me write it clearly here,  $\dot{\rho} - i H \rho$ , and there is a minus minus, so it is just minus  $i$ , there is just minus sign, 0 to  $t$ ,  $H$ ,  $\rho$ , commutator  $H$ ,  $\rho$ ,  $ds$ . We are assuming that the interaction Hamiltonian, interaction between the system and bath is captured by the interaction Hamiltonian. The interaction is weak and parameterized by a small parameter  $\lambda$ . So, the interaction Hamiltonian  $H_I$  depends directly on  $\lambda$ .

And  $\lambda$  is so big that  $\lambda^2$ , any term above  $\lambda^2$  can be neglected. So, we can stop this evolution or we can keep the dynamical equation up to second order in the interaction Hamiltonian. So, we don't need to go beyond this term. Another thing, the interaction Hamiltonian,  $H_I$ , can always be written as the operator acting on the system Hilbert space,  $A_\alpha$  tensor operator acting on bath Hilbert space  $B_\alpha$  and sum over  $\alpha$ . Any operator acting on  $H_s$  tensor  $H_b$  can be written in this form, for appropriate choice of  $A_\alpha$  and  $B_\alpha$ .

And let us assume that  $A_\alpha$  and  $B_\alpha$  are Hermitian, so  $A_\alpha^\dagger = A_\alpha$  and  $B_\alpha^\dagger = B_\alpha$ , one assumption we have, here for the open system dynamics is that bath is completely random. What does it mean is if we have the

state of the bath as the rho B initial state, then the expectation value of all the bath operators B alpha will be 0. So, it is a maximally random state. The bath is always in a maximally random state so that no information can be extracted from the bath. It means the bath operators we have used in the expansion of the Hamiltonian, the interaction Hamiltonian, the expectation value of those bath operators is zero.

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$$\begin{aligned} \dot{\rho}_I &= -i [H_I, \rho_I] \\ \rho_I(t) &= \rho_I(\omega) - i \int_0^t [H_I(s), \rho_I(s)] ds \\ \dot{\rho}(t) &= -i [H(t), \rho(t)] - \int_0^t [H(s), [H(s), \rho(s)]] ds \\ &= -i [H(t), \rho(t)] - \int_0^t [H(s), [H(s), \rho(s)]] ds \\ H_I &= \sum_{\alpha} A_{\alpha} \otimes B_{\alpha} \quad \begin{aligned} A_{\alpha}^{\dagger} &= A_{\alpha} \\ B_{\alpha}^{\dagger} &= B_{\alpha} \end{aligned} \\ &\rightarrow \text{Bath is Random.} \end{aligned}$$

This is what we will call as the bath is completely random. We can from here, we can calculate the interaction Hamiltonian in the interaction picture, which is  $R H_I R^\dagger$  where  $R$  is exponential of  $i H_S t$  plus  $H_B t$ . So,  $H_S$  and  $H_B$  commute. So, we can always write  $R$  to be exponential of  $i H_S t$  times exponential tensor exponential of  $i H_B t$  which is equal to which can be called  $R_S$  tensor  $R_B$ . From here we can calculate  $H_I(t)$  as sum over alpha  $R_S A_{\alpha} R_S^\dagger$  tensor  $R_B B_{\alpha} R_B^\dagger$ . Where  $R_S$  and  $R_B$  are the exponential of  $i H_S t$  and exponential of  $i H_B t$  respectively for the system and the bath.

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$$\begin{aligned} \text{Tr}[\rho_B(\omega) B_{\alpha}] &= \langle B_{\alpha} \rangle = 0 \\ H_I(t) &= R H_I R^\dagger \\ H_I(t) &= \sum_{\alpha} R_S A_{\alpha} R_S^\dagger \otimes R_B B_{\alpha} R_B^\dagger \\ &\rightarrow R_B B_{\alpha} R_B^\dagger = B_{\alpha}(t) \\ &\rightarrow R_S A_{\alpha} R_S^\dagger = A_{\alpha}(t) \end{aligned} \quad \left. \begin{aligned} R &= \exp(i(H_S + H_B)t) \\ &= \exp(i H_S t) \otimes \exp(i H_B t) \\ &= R_S \otimes R_B \end{aligned} \right\}$$

Let us call  $R_B = B^\dagger R B$  to be  $B^\dagger$ , the time dependent bar operators and similarly  $R_S = A^\dagger R S A$  equals  $A^\dagger$  as the system operators, so  $H_I(t)$  can be written as  $\sum_\alpha A_\alpha(t) B_\alpha(t)$ . Next is the Born approximation. In open system dynamics, typically we assume that the bath is so big as compared to the system that the state of the bath does not change just because it is interacting with the system. On the other hand, the system is very very small as compared to the bath. So, it will see some changes which will be calculated in the dynamical equation. So, Born approximation states that  $\rho_{SB}(t)$  the total state of the system and bath at time  $t$  can always be approximated as state of the system at time  $t$  tensor the state of the bath which is constant throughout the dynamics.

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→ Born approximation

$$\rho_{SB}(t) \approx \rho_S(t) \otimes \rho_B$$

$$\Rightarrow \dot{\rho}_S = \text{Tr}_B \left[ \dot{\rho}_{SB} \right] = -i \text{Tr}_B \left[ H_I(t), \rho_S(t) \otimes \rho_B \right] - \int_0^t ds \left[ H_I(s), [ H_I(s), \rho_S(s) \otimes \rho_B ] \right]$$

So, let me restate that the Born approximation says that the bath is so large as compared to the system that the state of the bath does not change as a result of the interaction with the system. So, the state of the bath remains same throughout the dynamics but the state of the system changes with time. So, total state of the system and bath can be approximated as product state between the system state  $\rho_S$  at time  $t$  tensor the steady state of the bath  $\rho_B$ . This implies that the  $\dot{\rho}_{SB}$  which was raised over  $\rho_{SB}$  the time derivative of the  $\rho_{SB}$  will be  $-i \text{Tr}_B H_I(t)$ , we are separating the subscript  $i$   $\rho_S(t)$  times the  $\rho_B$  minus  $0$  to  $t$   $ds H_I(t)$  commutator  $H_S \rho_S \otimes \rho_B$ . Let us look at the first term, the first term, the commutator is  $H_I(t) \rho_S(t) \otimes \rho_B$ . It should be  $\rho_S(0) \otimes \rho_B$  which is  $\sum_\alpha A_\alpha(t) \otimes B_\alpha(t) \rho_S \otimes \rho_B$  minus  $\sum_\alpha A_\alpha(t) \otimes B_\alpha(t) \rho_S \otimes \rho_B$  times  $\sum_\alpha A_\alpha(t) \otimes B_\alpha(t)$ .

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$$\begin{aligned} \text{Tr}_B \left[ H_I(t), \rho_S(t) \otimes \rho_B \right] &= \text{Tr}_B \left[ \left( \sum_\alpha A_\alpha(t) \otimes P_\alpha(t) \right) (\rho_S \otimes \rho_B) \right. \\ &\quad \left. - (\rho_S \otimes \rho_B) \left( \sum_\alpha A_\alpha(t) \otimes P_\alpha(t) \right) \right] \\ &= \sum_\alpha A_\alpha(t) \rho_S \otimes \text{Tr}_B [P_\alpha(t) \rho_B] \\ &\quad - \rho_S \sum_\alpha A_\alpha(t) \otimes \text{Tr}_B [P_\alpha(t) \rho_B] \end{aligned}$$

And then we take trace over the bath, trace over bath. When we take trace over bath, it becomes sum over alpha A alpha, rho s tensor trace over beta alpha t rho beta, rho B minus rho s, sum over alpha A alpha tensor trace over rho B B alpha t. So, this is the expectation value of the bath operator at time t and this is also the expectation value of the bath operator at time 0. Since the bath state does not evolve in time, it is in a steady state, so this expectation value is same as the expectation value at time 0 and since the bath is considered to be completely random, this tends to 0. Therefore, the first term itself goes to 0. And we are left with the simplified dynamical equation that is rho s dot equals trace over bath minus 0 to t ds, this is the integration, s is the integration parameter, H t commutator H s rho system at time s tensor rho bath. Our task is to simplify this equation and bring it to a simple form.

We can expand it to be trace over b minus 0 to t ds commutator of H t with H s rho s times rho B minus rho S rho B times H and this can be written in terms of, this can be written as minus 0 to t ds. There will be four terms because it's a commutator of one with the two terms. It will be ht hs rho s at s tends to rho b minus rho s at s rho b minus hs rho s at s tensor rho B times H t. This is the first term and the second term is minus H t rho s at s tensor rho B Hs. So, these are the four terms we have. So, we have to simplify all four terms to get the final expression for the dynamic equation.

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$$\begin{aligned} \dot{\rho}_S &= \text{Tr}_B \left[ \int_0^t ds \left[ H(s), \left[ H(s), \rho_S(s) \otimes \rho_B \right] \right] \right] \\ &= \text{Tr}_B \left[ \int_0^t ds \left[ H(s), H(s) \rho_S(s) \otimes \rho_B - \rho_S(s) \otimes \rho_B H(s) \right] \right] \\ &= \text{Tr}_B \left[ \int_0^t ds \left[ \left( H(s) H(s) \rho_S(s) \otimes \rho_B - H(s) \rho_S(s) \otimes \rho_B H(s) \right) \right. \right. \\ &\quad \left. \left. - \left( H(s) \rho_S(s) \otimes \rho_B H(s) - \rho_S(s) \otimes \rho_B H(s) H(s) \right) \right] \right] \end{aligned}$$

We take the first term alone, first term This is the first term I am writing here. So, the first term is  $H_t H_s \rho_s$  times  $\rho_B$ . We can expand  $H_t$  and  $H_s$  in terms of  $A_\alpha$  and  $B_\alpha$  and we get sum over alpha beta  $A_\alpha$  at time t tensor  $B_\alpha$  at time t,  $A_\alpha$  at time s tensor  $B_\alpha$  at time s,  $\rho_s$  at  $\rho_s$  at s tensor  $\rho_B$  and then there's a trace over bath, we will worry about that later. Now we use ABCD rule of tensor product. Let me remind you that rule.

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$$\begin{aligned}
 & \text{Tr} (H_t H_s \rho_s \otimes \rho_B) \\
 &= \sum_{\alpha\beta} (A_\alpha(t) \otimes B_\alpha(t)) (A_\beta(s) \otimes B_\beta(s)) \rho_s \otimes \rho_B \\
 & \quad (A \otimes B)(C \otimes D) = AC \otimes BD \\
 &= \sum_{\alpha\beta} A_\alpha(t) A_\beta(s) \rho_s \otimes B_\alpha(t) B_\beta(s) \rho_B \\
 & \quad \text{Tr}_B \\
 &= \sum_{\alpha\beta} A_\alpha(t) A_\beta(s) \rho_s \langle B_\alpha(t) B_\beta(s) \rangle
 \end{aligned}$$

If we have  $A$  tensor  $B$  times  $C$  tensor  $D$ , then we can write it as  $AC$  tensor  $BD$ . So, using that we can write it as alpha beta  $A_\alpha$  at time t  $A_\beta$  should be beta here, not alpha at time s,  $\rho_s$  at s tensor  $B_\alpha$  at t  $B_\beta$  at s. And  $\rho_B$ . Now if we take trace over  $B$  here, then we get sum over alpha beta,  $A_\alpha$  at t,  $A_\beta$  at s, and  $\rho_s$  times the expectation value of  $B_\alpha$  at t and  $B_\beta$  at t. So, the first term that is  $H_t H_s$  times  $\rho_s$   $\rho_B$  trace over, the partial trace over the bath degree of freedom results in an expression of expression in terms of  $A_\alpha$   $A_\beta$  and  $\rho_s$ . and the expectation value of the product of two bath operators,  $B_\alpha$  t and  $B_\beta$  s. And this is the two point correlation function in time of the bath operators. So,  $B_\alpha$  at t,  $B_\beta$  at s, which is trace  $B_\alpha$  at t,  $B_\beta$  at s and  $\rho_B$ . This is the two point correlation function of both operators at time t and at s. And let us call them  $C_{\alpha\beta}(t,s)$ . So, using this, we can write the dynamical equation  $\rho_s$  dot minus sum over alpha beta integration 0 to t d s.

There will be four terms here and that those will be  $A_\alpha$  at t  $A_\beta$  at s  $\rho_s$  at s times  $C_{\alpha\beta}$  and I'm just suppressing t and s, here the next term will be  $A_\beta$  of s  $\rho_s$  at s and  $A_\alpha$  at t  $C_{\alpha\beta}$ , that was with minus sign minus  $A_\alpha$  of t  $\rho_s$

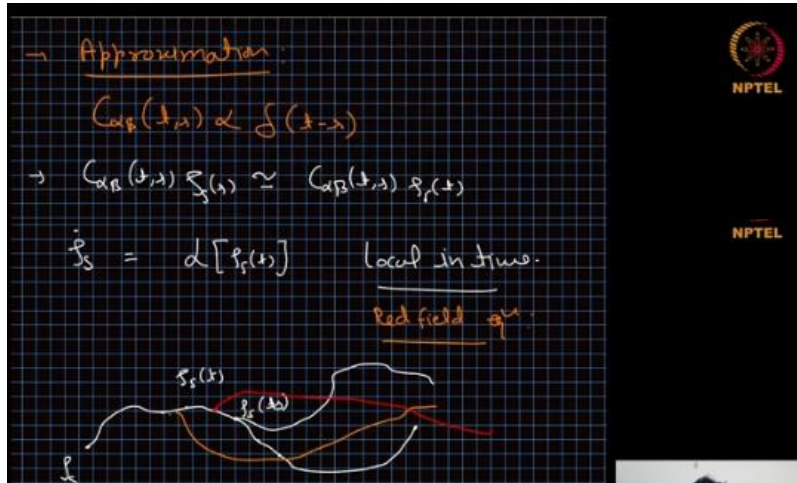
at  $s$   $A$  beta of  $s$ ,  $C$  beta  $C$  beta alpha plus rho  $s$  at  $s$   $A$  beta at  $s$   $A$  alpha at  $t$   $C$  beta alpha. So,  $C$  alpha beta is a function of  $t$   $S$ . So,  $C$  alpha beta is a function of  $t$   $S$ ,  $t$   $S$  and  $S$   $t$  and  $S$   $t$ . Okay so our dynamic equation in terms of rho  $s$  looks like this and you can see that the right hand side depends on the two point correlation function of the bath and the state rho  $s$  of the system along with the operators  $A$  alpha and  $A$  beta which acts on the system. So, in general, this equation is difficult to solve. To make it easy, we will apply some approximations and those approximations we will explain one by one.

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The first approximation we have is that  $C$  alpha beta  $t$   $s$  is  $\delta(t - s)$ .  $C$  alpha beta at  $t$   $s$  is proportional to  $\delta(t - s)$ . It is a delta function. What it means? It is an uncorrelated bath. It means the correlation in the bath operators at time  $t$  and at time  $t$  prime or  $s$  is 0. So, the correlation we can see only when the two operators are at the same time.

Therefore, we can write  $C$  alpha beta  $t$   $s$  times rho  $s$   $s$  to be same as  $C$  alpha beta  $t$   $s$  rho  $s$  at  $t$ . So, this is the property of a delta function that the delta function at any function at time  $s$  is same as the same delta function and the other function at time  $t$ . Using this, we can write that the dynamical equation for our system state as some super operator, some map acting on rho  $s$  of  $t$ . Unlike what we had so far here, where the rho  $s$  at time  $t$ , the derivative of rho  $s$  at time  $t$  depends on rho  $s$  at time  $s$ , some other time  $s$  and that  $s$  can take value from 0 to  $t$ , any value from 0 to  $t$ . But with this approximation that the bath correlation, the bath correlation dies very fast in time, we can make the dynamical equation local in time. This time local equation is called Redfield equation. And here the state at time  $t$  depends on the state at time  $t$ , but it considers the correlation functions from the earlier times also because the integration still depends from 0 to  $t$ . So, the equation is local in time in terms of the state.

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But it still has the information about the history of how the state was evolved. So, in that way, it's not a Markovian master equation. Markovian dynamics is something which does not depend on the history. So, if we have a quantum state  $\rho_s$ , let us say it's in some parameter space, and in time, it evolves, the state evolves using, taking some trajectory in the parameter space. So, there's some state  $\rho_s$ , this is  $\rho_s$  at time  $t$  and it takes this trajectory as.

If we have some state here at  $\rho_s$  at  $t_0$  and we forget about this system, we take another quantum system and prepare the state of the system in  $\rho_s$  at  $t_0$  and then we evolve it with this Hamiltonian, this open quantum system dynamics, Redfield equations or whatever dynamics we have. If it takes the same trajectory again, irrespective of where we started from, then it means the dynamics of the system does not depend on what path the system took to arrive at the state reverse  $t_0$  for any  $t_0$ . It means there is no information about the history of the evolution in that those kind of dynamics are called Markovian dynamics. But the Redfield equation in general does not satisfy this condition, in Redfield equation if we start from state  $\rho_s$  at  $t_0$  it might take something else, some different trajectory altogether. Similarly, from some other point if we start we will reach somewhere else, if we start from third point we will go somewhere else, so that the future dynamics of the quantum system depends on the history of the state. So, if we start from here we will get the original dynamics, if we start from somewhere else, then it will be, it will end up, we will end up getting some entirely different state, it is possible in Redfield equation. In order to make the Redfield, in order to convert the Redfield equation into Markovian dynamics, we need to make some further simplifications.

One of the simplification is that we take  $t$  equals 0 to  $t$  equals minus infinity. That is, we say that our dynamics does not start from  $t$  equals 0, but it starts from  $t$  equals minus  $t$  tending to minus infinity. And we can say that the interaction Hamiltonian for  $t$  less than 0 is just 0. So, there is no Hamiltonian or the Hamiltonian, the interaction between the system and bath before the time  $t$  equals 0 was 0 and after the time 0 it was some  $H_I$  was given by sum over alpha  $A_\alpha(t) \otimes B_\alpha(t)$  for  $t$  greater than or equal to 0 and for  $t$  less than 0, it was the interaction Hamiltonian is 0. So, there is no interaction between the before  $t$  equals 0 and the interaction Hamiltonian is given by this after  $t$  equals 0.

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$$\begin{aligned} &\rightarrow t=0 \rightarrow t \rightarrow -\infty \\ &H_I(t < 0) = 0 \\ &H_I = \sum_{\alpha} A_{\alpha}(t) \otimes B_{\alpha}(t) \quad t \geq 0 \\ &\frac{d\rho_s}{dt} = -\int_0^t ds \left[ \dots \right] + 0 = -\int_0^t ds \left[ \dots \right] - \int_{-\infty}^0 ds \cdot 0 \end{aligned}$$

It means we can write  $d\rho_s$  over  $dt$  to be 0 to  $t$   $ds$  means the factor we had calculated the expression plus 0 because the interaction is written as 0. This can be written as minus 0 to  $t$   $ds$  times the factor plus 0 to minus infinity to 0 minus sign here times  $ds$  times 0. We can write it from minus infinity to infinity  $t$   $ds$  times the expression in terms of the interaction Hamiltonian  $H_I$  and  $H_I$  is given by these two conditions that it is zero before  $t$  equals zero and it is given by this expression for  $t$  greater than or equal to second simplification we make is that we define a parameter  $\tau$  such that  $s$  is  $t$  minus  $\tau$ . This implies that when  $s$  equals  $t$ , that is the upper limit of the integration, then this would imply that  $\tau$  is 0. And when  $s$  tending to minus infinity, then  $\tau$  tending to infinity.

So, we have defined  $\tau$  as a function of  $s$  or  $s$  as a function of  $\tau$  such that when  $s$  is  $t$  then  $\tau$  is 0 and when  $s$  is minus infinity then  $\tau$  is infinity. So, the integration limit from minus infinity to infinity will become minus of  $d\tau$  0 infinity to 0 and that will be 0 to infinity  $d\tau$ . These two simplifications put together will convert the Redfield equation into a Markovian equation. And we get the dynamic  $\rho_s$  dot  $t$  to be minus 0 to infinity  $d\tau$   $H$  of  $t$  commutator  $H$  of  $t$  minus  $\tau$   $\rho_s$  of  $t$  tensor  $\rho_b$ . So, this is our



dynamical equation when we substitute  $s$  with  $t$  minus  $\tau$  and we assume the bath correlation functions are fast decay. This is a Markovian master equation.

And this we reached by using Born approximation also that is also called Born Markovian master equation.

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②  $s = t - \tau \Rightarrow s \rightarrow t \rightarrow \tau = 0$   
 $s \rightarrow -\infty \Rightarrow \tau \rightarrow \infty$   
 $\int_{-\infty}^{\infty} ds = - \int_{\infty}^0 d\tau = \int_0^{\infty} d\tau$   
 $\dot{\rho}_s(t) = - \int_0^{\infty} d\tau \text{tr}_B \left[ H(t), [H(t-\tau), \rho_s(t) \otimes \rho_B] \right]$   
 $\rightarrow$  Markovian master eqn.