

FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

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Open Quantum Systems: Introduction - Part 03

To simplify the dynamical equation further, let us define the projectors P_ϵ for a non-degenerate system Hamiltonian H_S . Non-degenerate means the eigenvalues do not repeat for the Hamiltonian H_S for that P_ϵ will be just $|\psi_\epsilon\rangle\langle\psi_\epsilon|$ where $H_S |\psi_\epsilon\rangle = \epsilon |\psi_\epsilon\rangle$ that is $|\psi_\epsilon\rangle$ are the eigenstate of the Hamiltonian H_S with corresponding energy ϵ . But if the Hamiltonian is degenerate then we can have more than one eigenstate corresponding to the same energy in the sum over all those projectors having the same energy, we are calling it with just one projector P_ϵ . So, P_ϵ is the eigen projector of the system of H_S and we can write $H_S P_\epsilon = \epsilon P_\epsilon$. So, we are defining the projectors P_ϵ in this way and sum over ϵP_ϵ will be identity because this will contain all the projected rank 1 projectors over the eigenstates of H_S and H_S is the Hermitian operator.

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$$\dot{\rho}_S(t) = -\int_0^t dt' \text{tr}_E \left\{ H(t), [H(t-t'), \rho_S(t') \otimes P_E] \right\}$$

→ Markovian master eq.
 Born-Markov Master eq.

$$\Pi_\epsilon = \sum_c |c\rangle\langle c| \quad H_S |c\rangle = \epsilon |c\rangle$$

So, the eigenvectors forms a complete and orthonormal basis and this becomes a completeness relation. Next, we define a α of ω to be $P_\epsilon A P_{\epsilon'}$ sum over ϵ and ϵ' such that $\epsilon - \epsilon' = \omega$. So, we take the projector of A from the left on P_ϵ on the right on $P_{\epsilon'}$ such that the difference between ϵ' and ϵ is ω . So, we take the sum over all those things and we call it as A_α . We can see that A_α^\dagger becomes $\rho_S(\epsilon) \rho_S(\epsilon')$

epsilon prime A alpha pi epsilon, all three pi epsilon pi epsilon prime and A alpha, all three are Hermitian but when we take the Hermitian conjugate, they change their positions but they remain the same.

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$\rightarrow \Pi_\epsilon = \sum_c |\psi_\epsilon\rangle \langle \psi_\epsilon|$ $H_\epsilon |\psi_\epsilon\rangle = \epsilon |\psi_\epsilon\rangle$
 $H_\epsilon \Pi_\epsilon = \epsilon \Pi_\epsilon$
 $\sum_\epsilon \Pi_\epsilon = \mathbb{1} \rightarrow$ Completeness Relation.
 $\rightarrow A_\alpha^\dagger(\omega) = \sum_{\substack{\epsilon, \epsilon' \\ \epsilon' - \epsilon = \omega}} \Pi_\epsilon A_\alpha \Pi_{\epsilon'}$

So, this is our dagger of Hermitian conjugate of A alpha omega and this is nothing but A alpha of minus omega. Hs of A alpha omega will be Hs A alpha of omega minus A alpha of omega Hs. Here this will be Hs, sum over epsilon, epsilon prime pi epsilon A alpha pi epsilon prime minus sum over epsilon epsilon prime pi epsilon A alpha pi epsilon prime Hs Hs acting on pi epsilon will give us epsilon. Hs acting on pi epsilon prime will give us epsilon prime.

So, we get epsilon minus epsilon prime the A alpha of omega, which is minus of omega A alpha of omega. Similarly, Hs A alpha dagger omega will be omega A alpha of omega. We can see such examples of examples of such operators. For example we have the a and a dagger, the annihilation and creation operators for a harmonic oscillator. From here we have number operator a dagger a, which is n, the commutation of a and a dagger is one. Now from here we see that a dagger a and a is minus a and a dagger a with a dagger is a dagger and this is same as here just omega becomes 1. So, if we had a Hamiltonian Hs to be h bar omega times N plus half that is the Hamiltonian of the simple harmonic oscillator.

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$\rightarrow A_\alpha(\omega)^\dagger = \sum_{\epsilon, \epsilon'} \Pi_{\epsilon'} A_\alpha \Pi_\epsilon = A_\alpha(-\omega)$
 $[H_\epsilon, A_\alpha(\omega)] = H_\epsilon A_\alpha(\omega) - A_\alpha(\omega) H_\epsilon$
 $= H_\epsilon \sum_{\epsilon'} \Pi_{\epsilon'} A_\alpha \Pi_{\epsilon'} - \sum_{\epsilon'} \Pi_{\epsilon'} A_\alpha \Pi_{\epsilon'} H_\epsilon$
 $= (\epsilon - \epsilon') A_\alpha(\omega)$

H_S with a will be $\hbar \omega$ we are putting to be 1 if we put it to be 1 it will be minus ωa and H_S with a dagger will be ωa^\dagger . This is a very well known example of such operators A_α ω and A_α ω dagger. Since $\sum_\epsilon \pi_\epsilon \pi_{\epsilon'} = 1$ identity that is the completeness relation, say that A_α is $\sum_\epsilon \pi_\epsilon A_\alpha$ ω , $\sum_\epsilon \pi_{\epsilon'} A_\alpha$ ω . And this can be written as \sum_ω and $\sum_\epsilon \pi_\epsilon - \pi_{\epsilon'} = \omega$. $\pi_\epsilon a^\dagger \pi_{\epsilon'}$ and which becomes $\sum_\omega a^\dagger$ ω . In that way A_α can be decomposed as the combination of A_α ω for all the ω .

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$[H_S, A_\alpha^\dagger(\omega)] = \omega A_\alpha(\omega)$
Examples: $a, a^\dagger \rightarrow a^\dagger a = N$
 $[a, a^\dagger] = 1$ $H_S = \hbar \omega (N + \frac{1}{2})$
 $[a^\dagger a, a] = -a \Rightarrow [H_S, a] = -\omega a$
 $[a^\dagger a, a^\dagger] = a^\dagger$ $[H_S, a^\dagger] = \omega a^\dagger$

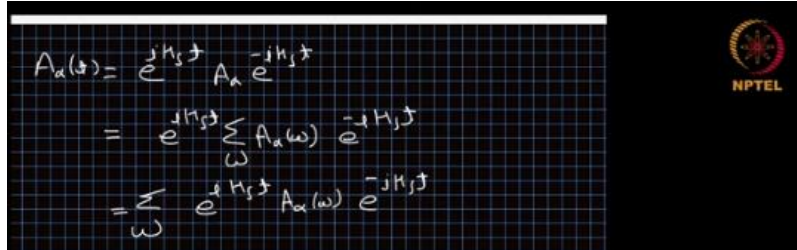
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$\sum_\epsilon \pi_\epsilon = 1$
 $A_\alpha = \sum_\epsilon \pi_\epsilon A_\alpha \sum_{\epsilon'} \pi_{\epsilon'}$
 $= \sum_\omega \sum_{\epsilon, \epsilon' = \omega} \pi_\epsilon A_\alpha \pi_{\epsilon'}$
 $= \sum_\omega A_\alpha(\omega)$

Now A_α of t which is exponential of $i H_S t$ α exponential of minus $i H_S t$. A_α of t was the operator, system operator in the interaction picture and by definition it is given by exponential of $i H_S t$ α exponential minus $i H_S t$. This can be written as exponential of $i H_S t$ $\sum_\omega A_\alpha$ of ω exponential minus $i H_S t$, summation can be taken out, \sum_ω exponential of $i H_S t$ A_α of ω exponential of minus $i H_S t$. This expression exponential of $i H_S t$ A_α of ω exponential minus $i H_S t$, it can be expanded as A_α of ω , plus $i H_S A_\alpha$ of

omega times t plus i t square over 2 Hs commutator Hs commutator A alpha omega and so on. This is called BCH expansion this is called BCH formula.

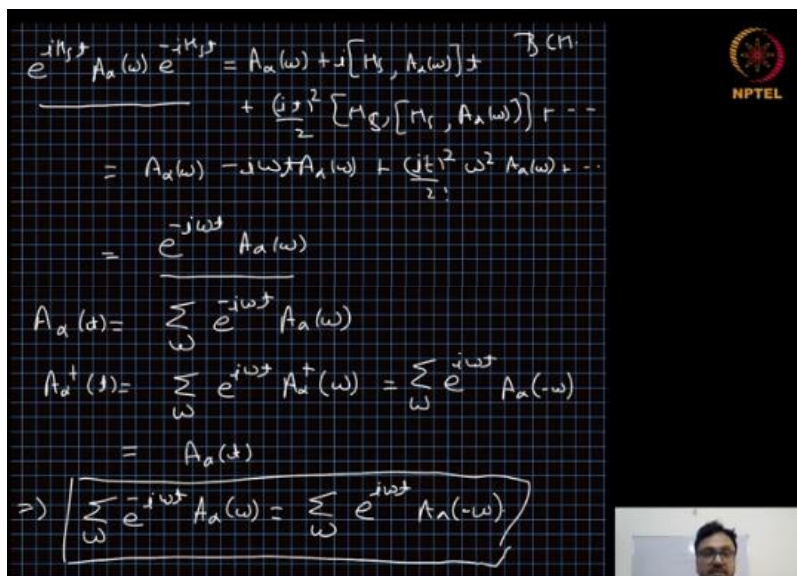
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The image shows a handwritten derivation on a grid background. It starts with the expression $A_\alpha(t) = e^{jH_S t} A_\alpha e^{-jH_S t}$. This is then written as $e^{jH_S t} \sum_{\omega} A_\alpha(\omega) e^{-jH_S t}$. Finally, it is rearranged to $\sum_{\omega} e^{jH_S t} A_\alpha(\omega) e^{-jH_S t}$. An NPTEL logo is visible in the top right corner of the slide.

And we can see that $H_S A_\alpha \omega$ is minus of ωA_α of ω . So, the whole thing can be written as A_α of ω plus or minus $i \omega A_\alpha$ of ω plus $i t$ square over 2 factorial ω square A_α of ω and so on. We combine it all, it becomes exponential of minus $i \omega t$, there is a t here sitting, A_α of ω . So, the whole expression, this complicated expression can be written in terms of exponential of $i \omega t$, A_α of ω and A_α of t is sum over ω , exponential of minus $i \omega t$, A_α of ω . Similarly, A_α^\dagger of t can be written as sum over ω exponential of $i \omega t$ A_α^\dagger of ω which is sum over ω exponential of $i \omega t$ A_α of minus ω .

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The image shows a handwritten derivation on a grid background. It starts with the BCH expansion: $e^{-j\omega t} A_\alpha(\omega) e^{j\omega t} = A_\alpha(\omega) + j[H_S, A_\alpha(\omega)]t + \frac{(jt)^2}{2} [H_S, [H_S, A_\alpha(\omega)]] + \dots$. This is then simplified to $A_\alpha(\omega) - j\omega t A_\alpha(\omega) + \frac{(jt)^2 \omega^2 A_\alpha(\omega)}{2!} + \dots$, which is recognized as $e^{-j\omega t} A_\alpha(\omega)$. Next, the adjoint action is shown: $A_\alpha(t) = \sum_{\omega} e^{-j\omega t} A_\alpha(\omega)$ and $A_\alpha^\dagger(t) = \sum_{\omega} e^{j\omega t} A_\alpha^\dagger(\omega) = \sum_{\omega} e^{j\omega t} A_\alpha(-\omega)$. Finally, it is concluded that $\sum_{\omega} e^{-j\omega t} A_\alpha(\omega) = \sum_{\omega} e^{j\omega t} A_\alpha(-\omega)$. An NPTEL logo is visible in the top right corner of the slide, and a small video inset of a person is visible in the bottom right corner.

And since $A_\alpha(t)$ is Hermitian, this is same as $A_\alpha(t)$. From here we can say sum over ω exponential of $-i\omega t A_\alpha(\omega)$ is same as sum over ω exponential of $i\omega t A_\alpha(-\omega)$. It may not seem so, but this is a huge improvement over, this is a huge simplification for our dynamical equation which will be apparent very soon. So, let us write the interaction Hamiltonian, sum over α and ω $A_\alpha(\omega)$ tensor $B_\alpha(t)$, becomes sum over α and ω $A_\alpha(\omega)$ exponential of $-i\omega t$, $A_\alpha(\omega)$ tensor $B_\alpha(t)$. From here, the dynamic equation ρ_s dot at time t becomes $-\int_0^t d\tau$, which is trace over bath H_i , H at time t , commutator H at time s , ρ_s tensor ρ_b and we can write it as $\int_0^t d\tau$ sum over α β ω ω' exponential of $-i\omega t$ exponential of $-i\omega' t$ $A_\alpha(\omega)$ $A_\beta(\omega')$ ρ_s tensor $A_\beta(\omega')$ times $C_{\alpha\beta}(t-\tau)$ minus τ comma t minus τ minus exponential of $-i\omega t$ minus τ , minus exponential of $-i\omega' t$ $A_\beta(\omega')$ ρ_s $A_\alpha(\omega)$ ρ_s of t times $C_{\beta\alpha}(t-\tau)$ at t plus Hermitian conjugate of the two term. So if we go back to our original equation after replacing the bath operators with the two point correlation functions.

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$$H_I = \sum_{\alpha, \omega} A_\alpha(\omega) \otimes B_\alpha$$

$$H_I(t) = \sum_{\alpha, \omega} e^{-i\omega t} A_\alpha(\omega) \otimes B_\alpha(t)$$

$$\dot{\rho}_s(t) = - \int_0^t d\tau \text{Tr}_B [H_I(t), [H_I(\tau), \rho_s(t-\tau) \otimes \rho_B]]$$

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$$G_s(t) = -\int_0^\infty dz \text{Tr}_E \left[H(t), [H(z), \rho_S(z) \rho_B] \right]$$

$$= \int_0^\infty dz \sum_{\alpha \beta} \left[e^{-i\omega(t-z)} e^{-i\omega'z} A_\alpha(\omega) \rho_S(t) A_\beta(\omega') C_{\alpha\beta}(z, t) \right. \\ \left. - e^{-i\omega(t-z)} e^{-i\omega'z} A_\beta(\omega') A_\alpha(\omega) \rho_S(t) C_{\alpha\beta}(t-z, t) + \text{H.c.} \right]$$

And we substitute A alpha of t and A beta of s. First we replace by t minus tau and then we replace A alpha of t as sum over omega exponential of minus i omega t A alpha of omega. Then we get this equation and we are using a Hermitian conjugate so that we don't need to repeat the terms again and again. Hermitian conjugate will be the complex conjugate of the complex numbers and Hermitian conjugate of the operators. Now let us define to make it this expression look a little bit more simpler. Let us define capital gamma alpha beta of omega as zero to infinity d tau exponential of i omega tau, the expectation value of B alpha t B beta of t minus tau.

We are defining the Fourier transform of the two point correlation functions and gamma alpha beta. Since rho B is time independent, that is a steady state. This was the Born approximation that the state of the bath does not change with time. So, it's time independent, so it's a steady state. The bath correlation functions, B alpha of t, B beta of t minus tau is same as B alpha of tau, B beta of zero.

So, the time translation does not matter here so these two are same so the bath correlation function the Fourier transform gamma alpha beta omega does not depend on t it depends only on tau and the omega. Using this we can write rho s dot t to be, so what we have done is we have consumed omega tau this term from first expression and second expression, we have consumed this term with C alpha beta to get the gamma alpha beta. So, with this we have a little bit simplified version of the equation and that is omega omega prime sum over alpha beta a alpha, exponential of minus i omega minus omega prime t gamma alpha beta omega A beta omega A alpha omega prime rho s at time t A alpha omega prime. So, we have replaced the integration over tau.

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$$\text{let } G_{\alpha\beta}(\omega) \sim \int_0^\infty dz e^{i\omega z} \langle B_\alpha(t) B_\beta(t-z) \rangle$$

$\rightarrow \rho_B \rightarrow \text{time-independent steady state}$

$$\langle B_\alpha(t) B_\beta(t-z) \rangle = \langle B_\alpha(z) B_\beta(0) \rangle$$

$$\Rightarrow \dot{\rho}_{\alpha\beta}(t) = \sum_{\omega, \omega'} \int_{-\infty}^t e^{-i(\omega-\omega')\tau} \left[\Gamma_{\alpha\beta}(\omega) A_{\beta}(\omega) \rho_{\alpha\beta}(\tau) A_{\alpha}(\omega) - A_{\alpha}(\omega) A_{\beta}(\omega) \rho_{\alpha\beta}(\tau) \Gamma_{\alpha\beta}(\omega) + h.c. \right]$$

$$\Rightarrow \dot{\rho}_{\alpha\beta}(t) = \sum_{\omega, \omega'} \int_{-\infty}^t e^{-i(\omega-\omega')\tau} \left[\Gamma_{\alpha\beta}(\omega) A_{\beta}(\omega) \rho_{\alpha\beta}(\tau) A_{\alpha}(\omega) - A_{\alpha}(\omega) A_{\beta}(\omega) \rho_{\alpha\beta}(\tau) \Gamma_{\alpha\beta}(\omega) + h.c. \right]$$

$\omega, \omega' \sim 10^{14} - 10^{15} \text{ Hz}$
 $t \sim 10^{-10} - 10^{-9} \text{ sec.}$

We have observed the integration over tau in the definition of gamma alpha beta and we get this expression. Now, consider the expression exponential of minus i omega minus omega prime t. This expression depends on the frequency of the system omega and omega prime and the time of evolution t. So, if the frequencies are optical frequencies, let us say, so omega if it is 10 to the power 14 to 10 to the power 15 hertz and omega prime is also of the same order, time of the evolution is typically nanosecond or picosecond. So, it is between 10 to the power minus 10 to 10 to the power minus 9 seconds. So, the product of omega times t is a very large number and exponential of that very large number is a very, very fast oscillating term.

This term for these typical values will be a very, very fast oscillating term. So, the average effect of these terms on the evolution of the state will be nullified and the average will be 0. So, we will not see any dynamics of the system. But in the cases when omega equals omega prime or very close to it, then these terms can be discarded. And in such cases, we get rho s dot, t becomes sum over omega alpha beta because we are using omega equals omega prime and the first term is discarded gamma alpha beta omega A beta omega rho s t A alpha omega minus A alpha omega prime A beta omega rho s of t plus Hermitian conjugate. So, wherever we had omega and omega prime we have replacing omega prime with omega. So, in general the gamma alpha beta is a complex number. So, we can write gamma alpha beta omega as half times gamma alpha beta omega which is a real number plus i S alpha beta where S alpha beta is also a real number. So, gamma alpha beta becomes capital gamma alpha beta omega plus gamma alpha beta omega star which is given by minus infinity to infinity d tau exponential of i omega tau B alpha tau B beta zero and we can write rho s dot to be minus i H IS and we will define what it is rho s plus d of rho s at t times t, where HLS is the Hamiltonian for lamb shift. It is called lamb shift Hamiltonian. It is given by alpha beta A dagger alpha omega A beta omega sum over alpha and beta and omega. And this is called lamb shift

Hamiltonian. Lamb shift is the shift in the energy levels of the quantum system posed by its interaction with the bath system.

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$$\dot{\rho}_S(t) = \sum_{\alpha\beta} \left[\Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_S(t) A_\alpha^\dagger(\omega) - A_\alpha^\dagger(\omega) A_\beta(\omega) \rho_S(t) \right) + H.c. \right]$$

$$\rightarrow \Gamma_{\alpha\beta}(\omega) = \frac{1}{2} \gamma_{\alpha\beta}(\omega) + i S_{\alpha\beta}$$

$$\gamma_{\alpha\beta} = \Gamma_{\alpha\beta}(\omega) + \Gamma_{\alpha\beta}^*(\omega)$$

$$= \int_{-\infty}^{\infty} dz e^{i\omega z} \langle R_\alpha(z) B_\beta(0) \rangle$$

$$\Rightarrow \dot{\rho}_S = -i [H_{LS}, \rho_S] + \mathcal{D}(\rho_S(t))$$

$$H_{LS} = \sum_{\alpha\beta} \frac{S_{\alpha\beta}}{\omega} \underbrace{A_\alpha^\dagger(\omega) A_\beta(\omega)}_{\text{bath correlation}} \rightarrow \text{Lamb Shift}$$

And we can see that here $S_{\alpha\beta}$ is the information we are getting from the bath correlation function. And A_α and A_β are the operators of the system. So, this is the Hamiltonian of the system posed by the bath correlation functions. If the bath correlation is 0, then this term goes to 0. Then bath correlations are 0 only when, so this term will be 0 only when there is no interaction between system and the bath.

\mathcal{D} of ρ_S is called dissipator. So, this is a map acting on ρ_S and given by sum over ω , sum over $\alpha\beta$, $\gamma_{\alpha\beta}(\omega)$, $A_\beta(\omega) \rho_S(t) A_\alpha^\dagger(\omega)$, $A_\alpha^\dagger(\omega) A_\beta(\omega) \rho_S(t)$. So, this is the simplest and final form of the random dynamical equation we have now. First term, is the Lamb shift which is caused by the interaction of the system with the bath degree of freedom and the second term is the dissipator which results in the loss of the coherence and the quantum effect in the system. Both of these terms are coming purely because of the interaction of the system with the bath and let me remind you that this whole thing is in the interaction picture.

After solving this dynamic in the interaction picture, we can go back to the Schrodinger picture and find the dynamics of the state in that picture. Last remarks, it can be proven that if we consider matrix G , which contains $\gamma_{\alpha\beta}$. So, the $\gamma_{\alpha\beta}$

beta are the real numbers and for different alpha betas, we can make a matrix G. Then it can be proven that this is a positive semi-definite matrix. What does it mean?

It means G is Hermitian and the eigenvalues of G are always non-negative. It means G can be written as some unit free times U times U times d times U dagger where U is unitary and d is some diagonal matrix. And let us say these are gamma 1, gamma 2, gamma n. It means gamma alpha beta can be written as U alpha i D i j U dagger j beta and sum over i and j. This can be written as this is equal to sum over ij U alpha i u star beta j D ij is gamma i delta ij. And we can just remove the sum over j. Replace all the j's with i's and remove the delta function.

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$\rightarrow G = [\gamma_{\alpha\beta}] \rightarrow \text{true semi-definite.}$
 $G = G^\dagger \quad e_{ij}(G) \geq 0$
 $\Rightarrow G = U D U^\dagger ; D = \begin{bmatrix} \gamma_1 & & \\ & \gamma_2 & \\ & & \ddots \\ & & & \gamma_N \end{bmatrix}$

So, gamma i alpha beta is U alpha i U star beta i gamma i. Substituting it in the dynamical equation or in the dissipator, D of rho s becomes sum over n and omega gamma n Ln rho s Ln dagger minus Ln dagger Ln rho, anticommutator rho s. where Ln is defined as sum over alpha, U alpha, i, Ai. These are called in Lindblad operators. So, if we consider only the dissipative dynamics of the system and forget about the lamb shift, then rho dot can be written as sum over n gamma n Ln rho s Ln dagger minus half times Ln dagger Ln rho s anti-commutator.

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$$\Rightarrow \dot{\rho}_{\alpha\beta} = \sum_j U_{\alpha j} D_j (U^\dagger)_{j\beta} \rho$$

$$= \sum_j U_{\alpha j} U_{\beta j}^\dagger \dot{\rho}_j$$

$$D(\rho_j) = \sum_{n,\omega} \gamma_n \left[L_n \rho_j L_n^\dagger - \frac{1}{2} \{ L_n^\dagger L_n, \rho_j \} \right]$$

$$L_n = \sum_{\alpha} U_{\alpha j} A_{\alpha}(\omega) \rightarrow \text{Lindblad operators}$$

$$\dot{\rho}_j = \sum_n \gamma_n \left[L_n \rho_j L_n^\dagger - \frac{1}{2} \{ L_n^\dagger L_n, \rho_j \} \right]$$

\rightarrow Markovian Master eqⁿ

There is a half vector here missing. So, half times $L_n^\dagger L_n \rho$. So, this becomes our final dynamical equation of the system when it is interacting with a bath. We have made certain approximations, but with those approximations, we have achieved Markovian master equation for the dynamics of a system interacting with a bath. This is also called Lindblad master equation.