FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

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Week-11
Lecture-31

Open Quantum Systems: Optical Master Equation, Thermalization

In open quantum systems, so far we have only achieved the master equation, Lindblad master equation of the system and that is given by sum over n, gamma n Ln rho s Ln dagger minus half integration anti-commutator of Ln dagger Ln with rho s. So, where Ln are the Lindblad operators and gamma n are the dissipation terms. Next, we will consider an example of a two level system, preferably an atom interacting with a bath of electromagnetic field. So here our system is two level system, two level atom and the Hamiltonian of such system is given by h bar omega naught over two sigma z. Let me remind you sigma z is a two by two matrix one zero zero minus one. So, the eigenvalues are plus minus h bar omega naught over 2 and the eigenvectors as g which is 0 1 and e can be written as excited state is 1 0.

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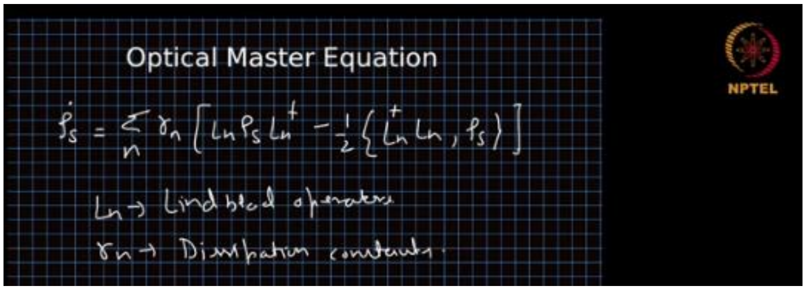

So, e is, e corresponds to h bar omega naught over 2 energy and g corresponds to h bar omega naught over 2 with negative sign. This is our system, our bath, is the bath of electromagnetic field. So we have electromagnetic field mode everywhere in the space time in the whole space and the system is interacting with the atom, the two level atom is interacting with that bath the interaction Hamiltonian H i is given by minus d dot e where d is the dipole moment of the atom, electric dipole moment, operator of the atom and E is the electromagnetic field operator, electric field operator. So if we have a dipole moment and there is an electric field present, the interaction between the dipole moment and the electric field is given by minus d dot e. We have used the same interaction to consider the interaction between the atom and the electromagnetic bath.

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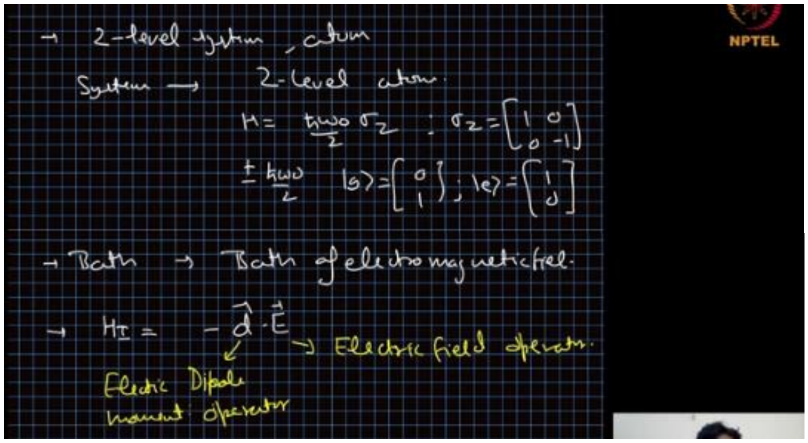

But d here now is the vector of operators and this is electric dipole moment operator of the atom and E is the electric field operator of the bath. Dipole moment operator d is given by the d vector times sigma minus plus d vector star times sigma plus, where d vector is a two-dimensional vector of complex numbers and sigma plus and minus are given by sigma x plus i sigma y over 2. Let me remind you sigma x is 0 1 1 0 and sigma y is 0 minus i i 0, hence where sigma plus minus becomes 0 1 1 0 plus plus minus 0 1 minus 1 0 over 2. So it becomes Sigma plus becomes 0 1 0 0 and Sigma minus becomes 0 0 1 0.

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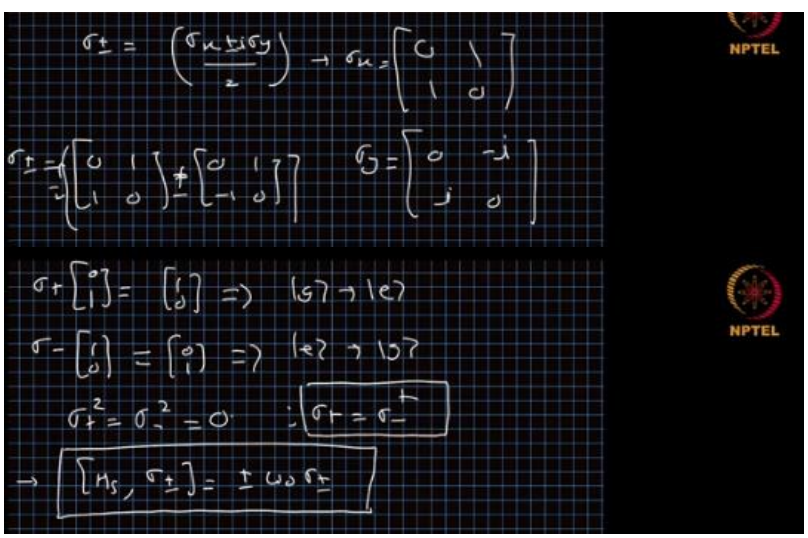

When we apply Sigma plus on the ground state, that is 0 1. We get one zero it means the ground state goes to excited state when we apply sigma plus and sigma minus, when we apply on the excited state we get the ground state sigma plus square equals sigma minus square equals zero. So, when we apply sigma plus or minus twice on any state we get just zero number is nothing on the other. Another interesting property is the commutator of the system Hamiltonian with sigma plus minus gives us plus minus omega naught sigma plus minus so in that way sigma plus minus are eigen operators of Hs this is why this relation. If you remember, in our treatment, in our derivation of the Lindblad operators, Lindblad master equation, we had A alpha omega, which satisfied something similar, something similar to this. And another thing, sigma plus and sigma minus are related.

The Hermitian conjugate of one gives us the other. Electric field operator is given by i sum over k sum over lambda one and two square root of two pi h bar omega k over V, we will explain each term soon, e lambda k vector b lambda k vector minus b lambda dagger k vector. Here lambda equals one and two represents the polarization of the light. k is the wave number, wave vector this represents the polarization but e lambda is the polarization vector. Lambda is index, the polarization. V is the volume of the cavity, we are assuming this electromagnetic mode in an optical cavity, so V is the volume of the cavity, so all these modes are solved assuming some finite boundary condition. So the volume, bk and bk dagger are the creation and annihilation operators corresponding to the polarization lambda and the wave vector k. So b lambda dagger k, creates a single photon in polarization lambda and the wave vector k. So k vector tells us the frequency and the direction of the propagation of the photon. So, lambda dagger k contains all that information in it, so photon is created with k vector and lambda attached to it.

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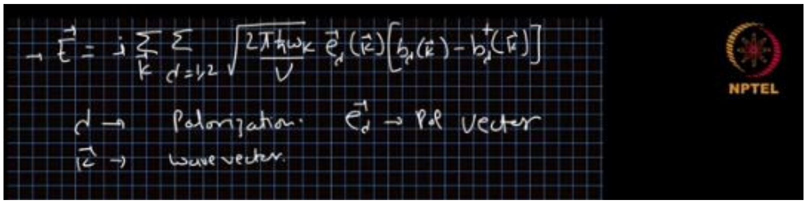

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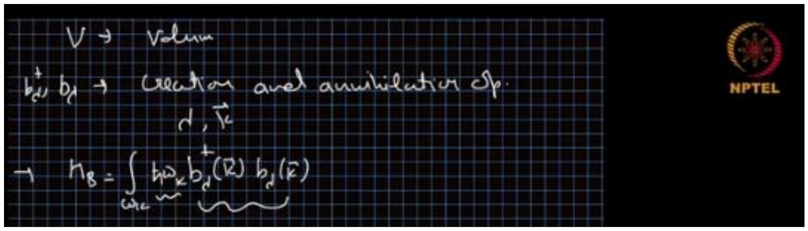

The free Hamiltonian of the bath Hb is given by b lambda k vector dagger b lambda k and the energy corresponding to it h bar omega k and integration over omega k for all the values. This is the most general Hamiltonian of the electromagnetic bath. It contains all the electromagnetic modes and the number of this is the number of operators of the given mode and the energy corresponding to it and the integration over the whole range. Now, from here, this is interesting that we, the commutation of Hb with b lambda dagger b lambda k and commutation of Hb with b lambda dagger k is minus omega k b lambda k and plus omega k b lambda dagger k. If the state of the bath rho b is a vacuum state that is, there is no photon in the bath there is no light then the bath correlation functions b lambda k b lambda prime dagger k prime will be delta of k minus k prime and delta of lambda lambda prime so unless the two polarizations are same and the two wave activities are same the expectation value is zero and the expectation value of b lambda prime dagger b lambda k is always 0 and when they are same when lambda and lambda prime are same then it is equal to 1. So from here we can calculate gamma alpha beta omega which was given as 0 to infinity d tau exponential of minus i omega tau and the expectation value of b alpha of tau b beta of 0 this can be calculated for the bath operators to be 2 over 3 h bar pi c cube delta alpha beta 0 to infinity d omega k omega k cube 0 to infinity ds exponential of minus i omega s so by substituting b alpha and b beta with b lambda prime dagger b lambda k we get the bath correlation function gamma, alpha, beta, omega to be this. Now, here is something interesting.

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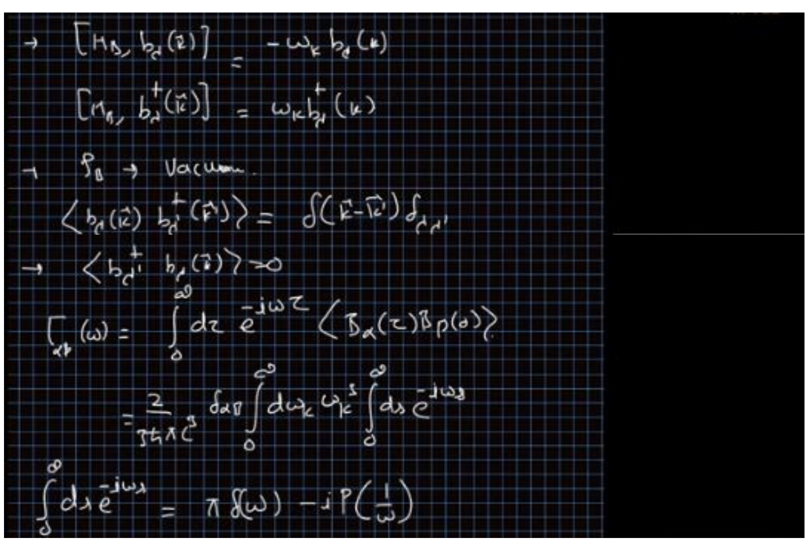

It is 0 to infinity ds exponential of minus i omega s can be written as pi delta of omega. So, this is delta function minus i p of 1 over omega, where p is the principal value function. Substituting this, we get gamma alpha beta omega to be 2 over 3 h bar pi c cube delta of alpha beta 0 to infinity d omega k omega k cube times pi delta of omega minus i principal value 1 over omega. So the first term will give us the gamma alpha beta and second term will give us the s alpha beta the coefficient for the lamb shift so uh the first term from here we can find the gamma alpha beta omega to be 2 over 3 h bar pi c cube delta alpha beta times 0 to infinity d omega k omega k cube pi delta of omega and this is simple when we have delta function and the integral, then we just substitute in the function we substitute omega k with omega and we get 2 over. So this is actually half times gamma 2 over 3 h bar pi and pi cancels p cube and we have omega k omega cube and there's a delta function delta of alpha beta we can take this factor 2 half and bring it here we get factor 4. So our gamma n let us say of omega becomes 4 over gamma becomes 4 over 3 h bar c cube omega cube similarly l of omega we can discard alpha beta because there is a delta function can be written as 2 over 3 h bar pi c cube d omega k omega k cube principal value of 1 over omega and this is nothing but 3 h bar pi c cube d omega k omega k cube over omega k minus omega principal value value of this. So for the case when the bath is in vacuum state, we saw that the dipole moment operator is d vector which determines the strength of the dipole moment times sigma minus plus d vector star sigma plus. For simplicity, we will use real vector then become d vector sigma plus plus sigma minus.

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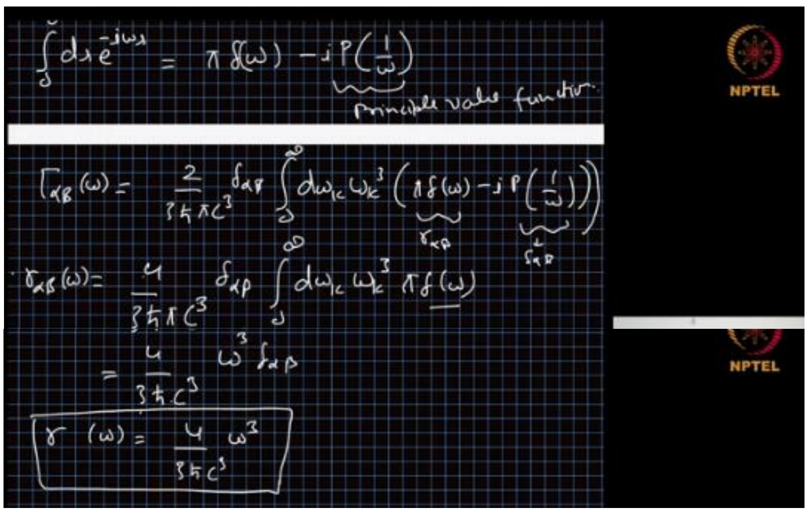

And our electric field operator is given as big expression with lambda and k and everything so our interaction Hamiltonian which is minus d dot e can be calculated from here and from there we can calculate the interaction Hamiltonian in the interaction picture we can substitute this interaction Hamiltonian in the interaction picture in the dynamical equation rho s dot which is minus 0 to infinity d tau h i of t h i of t minus tau rho s of t commutator and trace over bath. We saw earlier that this equation can be converted into the system operator acting on the rho s and the bath operator is converted into the bath correlation functions. We get the Lindblad equation, which is given by sum over n, gamma n ln rho ln dagger.

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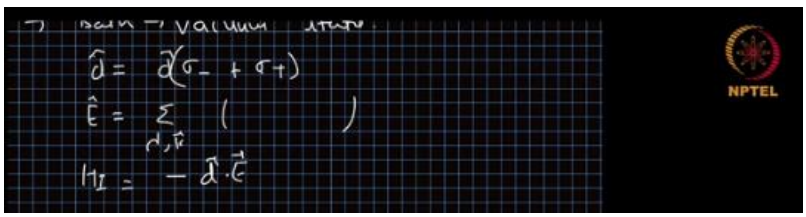

minus half anticommutator Ln dagger Ln it turns out that for the for this case where the atom the system is a two level atom and the bath is in the vacuum state we have only gamma n is equal to gamma naught which is 4 over 3 h bar omega cube over c cube d vector mod square and our Ln turns out to be sigma minus L0 is only one sigma minus and the Lindblad equation for two level atom interacting with electromagnetic bath in the vacuum state becomes gamma naught times sigma minus rho s sigma plus minus half sigma plus sigma minus rho minus half rho sigma plus sigma minus this is the Lindblad equation of two level atom interacting with electromagnetic bath in vacuum state. So, when a two-level atom interacts with an electromagnetic bath in vacuum state, the most profound phenomena we observe is the spontaneous emission.

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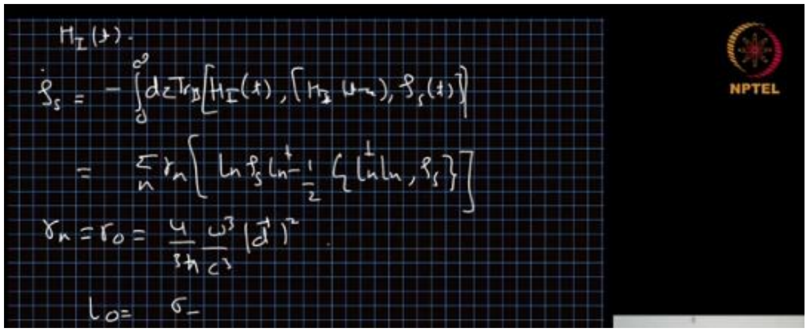

So, our atom left in the ground state will remain in the ground state forever. But if the atom is initially in the excited state, then it will decay to ground state. Then gamma naught becomes the spontaneous emission rate. So gamma naught is the spontaneous emission rate in that case. Other example is when the bath state is not a vacuum state, but it's the thermal state or Gibbs state. And Gibbs state is defined as exponential of minus beta H over Z, where beta is one over kBT, kB is the Boltzmann constant, T is the temperature and Z is defined as trace of exponential of minus beta H. So, that rho b is trace one.

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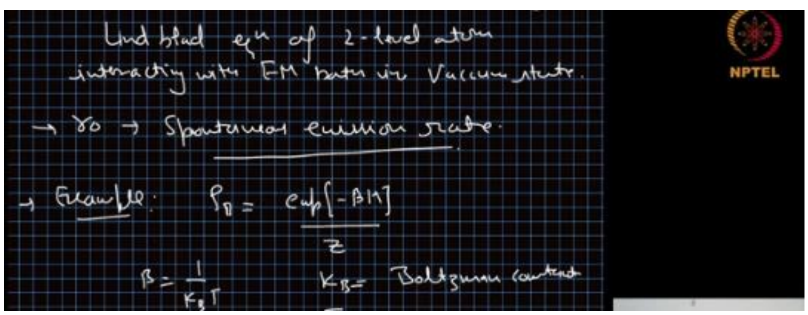

The average number of photons in a thermal distribution, a thermal state of a bath is given by N of omega. These are the number of photons, average number of photons having frequency omega and that is the expectation value of b k dagger b k, lambda sum over lambda where k is given by omega over c The magnitude of k is given by omega over c. So, this can be calculated to be 1 over exponential of beta h bar omega minus 1. From here, we can calculate the Lindblad coefficients gamma 1 and gamma 2 as 4 over 3 h bar c cube omega cube d mod square times 1 plus n of omega omega naught and omega 2 is 4 over 3 h bar c cube omega cube d mod square n of omega naught. Or we can write it as gamma naught, the spontaneous emission rate we had discussed for vacuum case, n of omega naught.

And this is gamma naught times N of omega. Where omega naught was the resonant frequency of the atom. And the Lindblad master equation can be written as gamma 1 times sigma minus rho s sigma plus. minus half sigma plus sigma minus rho s minus half rho s sigma plus sigma minus plus gamma 2 times sigma plus rho sigma minus minus half sigma minus sigma plus rho s minus half rho s sigma minus sigma plus. These equations are pretty straightforward and can be easily calculated after one understands the general derivation of the Lindblad-Master equation. The steps are very clear.

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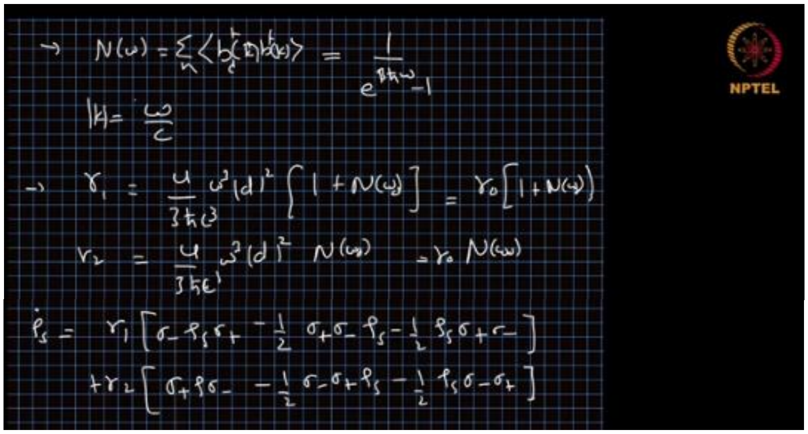

We have to just put this operator for the system, operator for the bath, the bath correlation functions and we arrive at this equation. Here we can see that N of omega goes to 0 for t tending to 0. So at zero temperature, the bath achieves the vacuum state. So the number of photons at omega will be zero. And in that case, gamma one will become gamma naught and gamma two will become zero.

And we retrieve the Lindblad-Master equation for the vacuum state. So when a two-level system interacts with the thermal bath, what happens to the final state of the system. So what is the steady state the system acquires when it interacts with the thermal bath. So instead of solving the dynamics given in the optical master equation formalism, we will start with the reverse question, if our our system is in the state exponential of minus beta H over Z where Z is given by trace of exponential of minus beta H and beta is 1 over kB T. kB is the Boltzmann constant, T is the temperature.

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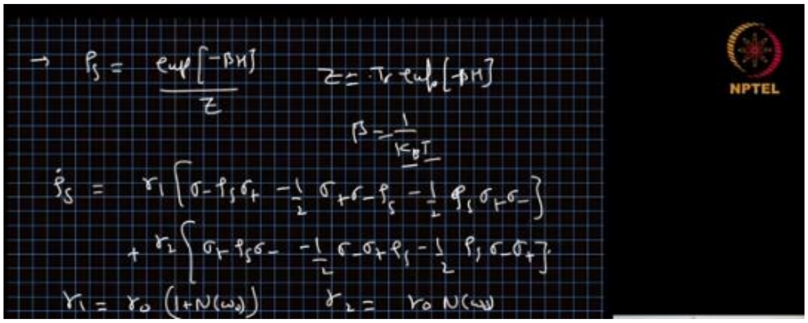

So, we have a state of the system which is the mathematical thermal state of the system. Now, if this is the initial state of the system, when you start interacting with the thermal bath, then what is the final state? That is the question we want to ask. That is, if we substitute rho s in the dynamical equation, rho s dot, then this is gamma 1, sigma minus, rho s, sigma plus, minus half, sigma plus, sigma minus, rho s, minus half, sigma, rho s, sigma plus, sigma minus, plus gamma 2 which is sigma plus rho s sigma minus minus half sigma minus sigma plus rho s minus half rho s sigma minus sigma plus where gamma 1 is gamma naught the spontaneous emission rate times 1 plus n of omega naught and gamma 2 is gamma naught times n of omega naught and n of omega naught is the thermal population of the state of the thermal bath. Now, we see that rho s is exponential of minus beta H over Z.

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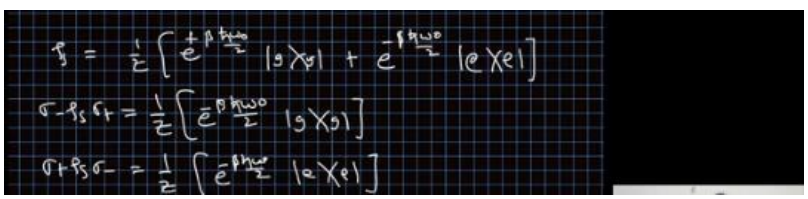

So, that is 1 over Z, it will be exponential of minus beta h bar omega naught over 2, times the minus plus the ground state plus exponential of minus beta h bar omega naught over 2 the excited state. The sigma minus rho s sigma plus will be sigma minus acting on the ground state gives us zero so we don't get anything sigma minus acting on excited state will give us the ground state.

So it becomes exponential minus beta h bar omega naught over two sigma minus e e sigma plus will be just g g. Similarly, sigma plus rho s sigma minus will be 1 over Z, it will be exponential of minus beta h bar omega naught over 2 e e. We can similarly calculate sigma plus sigma minus on rho s rho s, sigma minus sigma plus of rho s rho s, sigma plus sigma minus rho s, sigma minus sigma plus all the elements and we can substitute it here and we get rho s dot equals gamma naught 1 plus N of omega naught times exponential of minus beta h bar omega naught minus 1 rho th or rho s plus gamma naught times N of omega exponential of beta h bar omega naught minus 1 rho s after doing all these things this is what we get this can be simplified as gamma naught 1 plus n exponential of minus beta h bar omega naught minus 1 rho s plus or minus gamma naught N times exponential of beta h bar omega naught over 2 omega naught 1 minus exponential of minus beta h bar omega naught minus 1 times rho s. So that now we can take a few things common that is gamma naught and we can take exponential of minus beta h bar omega naught minus 1 common. And we are left with 1 plus n minus N times exponential of beta h bar omega naught times rho s. We recall that N is 1 over exponential of beta h bar omega naught minus 1.

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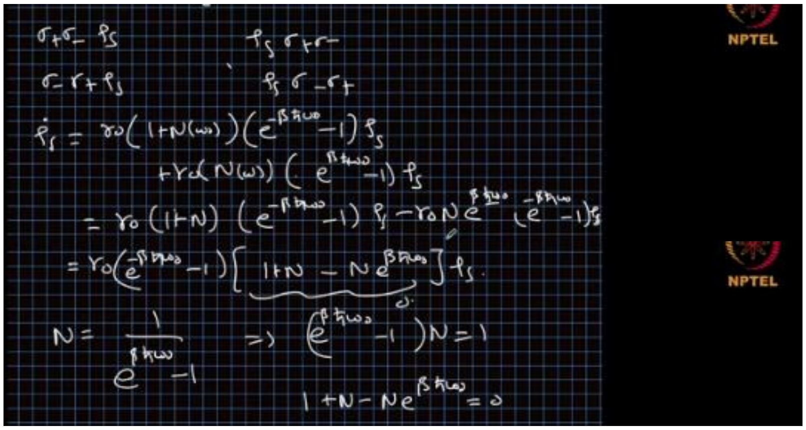

This implies that exponential of beta h bar omega naught minus 1 times N is 1. That is 1 plus N minus N exponential of beta h bar omega naught is 0. So this term is 0. We say that d rho s over dt is 0 if rho is the thermal state. This implies that the thermal state is a steady state. This kind of points towards the fact that if we have a two level system which is interacting with the thermal bath then the system itself acquires thermalization.

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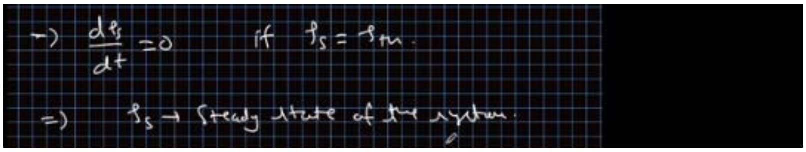

So, it acquires the thermal state eventually and that becomes the steady state of the system hence this process is called thermalization. Anything interacting with thermal bath will acquire the thermal state and this is in classical statistical mechanics it is called the equilibrium state.