FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

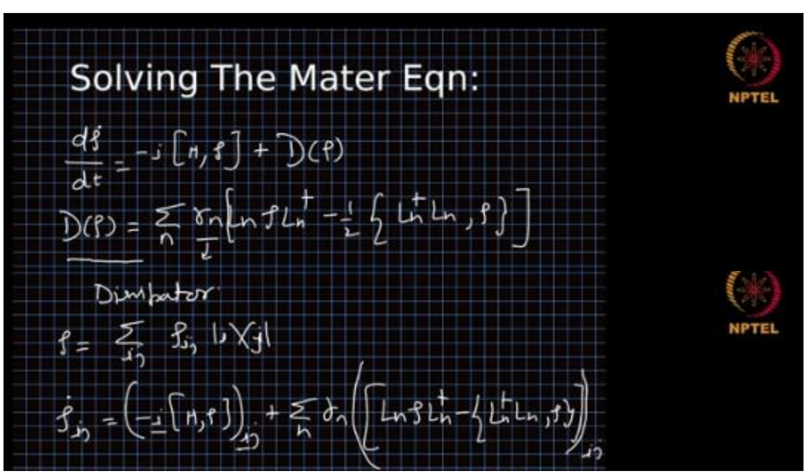
Dr. Sandeep K. Goyal
Department of Physical Sciences
IISER Mohali
Week-12
Lecture-32

Open Quantum Systems: Solving Master Equatons

In today's lecture we will talk about how to solve a given master equation, so master equation looks like the following d rho over dt equals minus i h bar h bar is one, so minus i commutator of H with rho where H is the Hamiltonian of the system and everything is system related, rho is the density matrix of the system at time t, H is the Hamiltonian of the system and we have D of rho where D is a super operator which is a dissipator. And in the Lindblad master equation, it is defined as sum over n gamma n Ln rho Ln dagger minus half anticommutator Ln dagger Ln with rho. This is the most general Lindblad master equation. We have gamma n's are the decay constants or Lindblad constants and D, this full thing is called dissipator.

So, our task is to solve this master equation. To see it, let us have rho as sum over ij, rho ij, these are the coefficients in the computational basis i out of j. So, ij is the computational basis. So, the time dependence, dependent part of the rho comes in the coefficient rho ij. So, we can write the master equation in terms of the coefficients rho ij and it reads rho as rho dot ij, dot is the time derivative, did I write so it's double here, it's not dot, so d over dt, we are writing as rho dot, rho ij minus i H commutators rho and the ijth element of that.

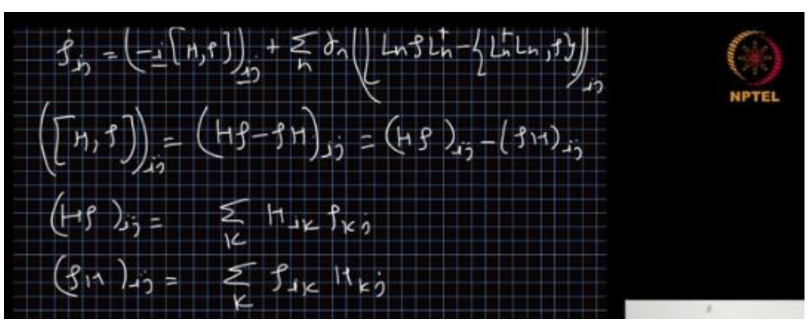
(Refer slide time: 3:18)



Don't confuse between this i and this i this is the square root of minus one and this i here is the index i could have used j and k but just out of habit I'm using ij, plus sum over n gamma n, Ln rho Ln dagger Ln is the are the Lindblad operators Ln dagger Ln rho and the ijth element of that So, if we have two matrices A and B and if we say A equals B, then the ijth element of A, every ijth element of A should be equal to ijth element of B. This is the property we are using in this equation. Now we have to calculate what is the ijth element of H commutator Rho and what is the ijth element of Ln rho Ln Dagger, what is the ijth element of Ln Dagger Ln rho, the anticommutator of this. So, let us start with the first one. Let us say we have H Rho commutator, which is H Rho minus Rho H and the ijth element of that will be ijth element of this, which will be H rho ijth element minus rho H ijth element.

Now, H rho ij element is sum over k H i k rho k j. This is the definition of the ijth element of the product of two matrices. Similarly, rho H ij, Sum over k, rho ik, H kj. We have used the same definition, just that the position of rho and H has changed. Now, how can we simplify this, is the question. So, let us see that what is H tensor identity, if we have H tensor identity and if we have ij kl element of it, how will it look like if we recall, our composite system lectures, where we were talking about the tensor products of two matrices then the ij klth element of this H tensor identity will be H ik and identity jl.

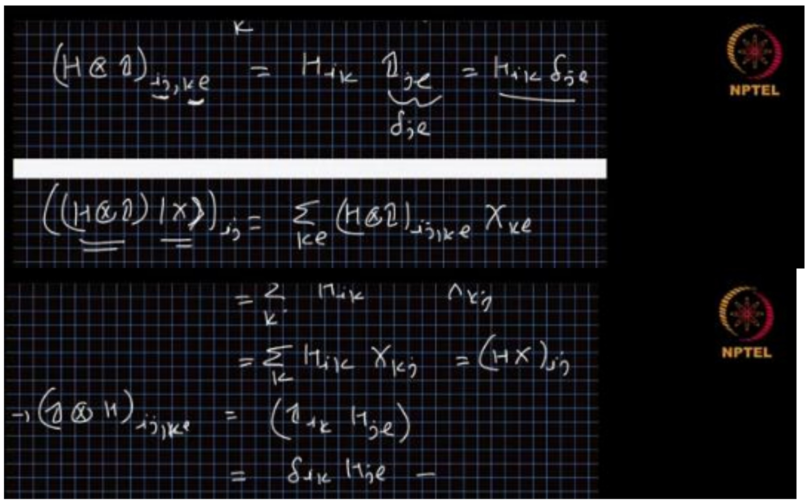
(Refer slide time: 4:06)



But identity is a diagonal matrix. So, i, j, l will be just delta jl. So, this is H, i, k, delta jl. If we say H tensor identity acting on a vector X and what is the ij th element of this? It will be sum over k, l H tensor identity, ij, kl and X, kl. This is a matrix acting on a vector. So, here we are identifying ij as one index and kl as another index.

So, it becomes the matrix acting on a vector equation. So, if we substitute this expression for H tensor I ijkl, we get sum over kl H ik delta jl X kl. Now, if we take sum over l, then we can replace all the l with j's. And we are left with sum over kl, H ik, X kj. So, H tensor identity acting on a vector X and the ij th element of that is as if we have taken H times X matrices.

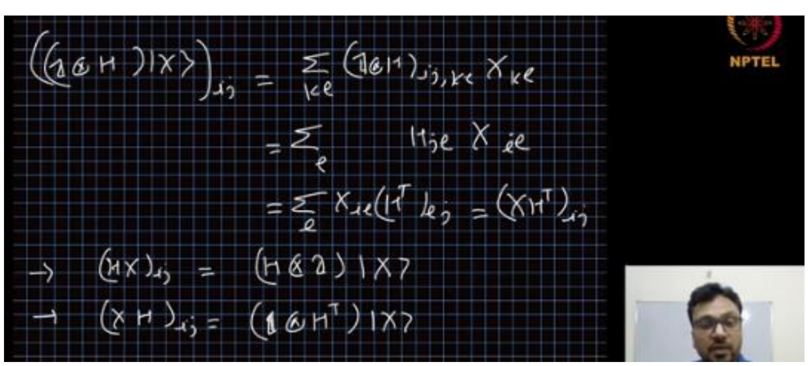
(Refer slide time: 7:44)



Similarly, if we have identity tensor, so this is one thing, this is another. Identity tensor H ijkl element will be I ik H jl and this is delta ik H jl. Identity tensor H acting on vector X. ij th element of that will be sum over kl. Identity tensor H, ij, kl and X, kl. The same thing we are doing what we did in the previous example. So, here again, we substitute for identity tensor H, ijkl with this expression and we get sum over kl, delta ik, H jl, X kl.

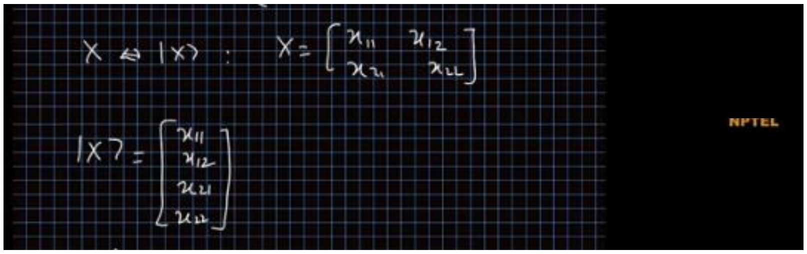
Now we can sum over k and replace all the ks with is. We remove k from here, delta we remove from here and k becomes i. So, this becomes sum over l X il H transpose lj. That is X H transpose ij. So, I tensor H acting on vector X and the ij element of that is X times H transpose and ij th element of that.

(Refer slide time: 8:56)



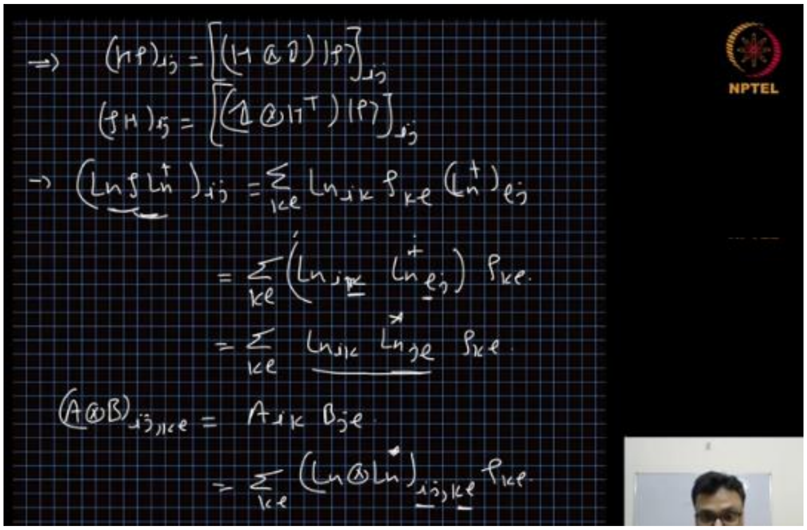
So, what we have established here is, if we have matrices H and X, H times Xij, this can be written as H tensor identity acting on the vector X, and H transpose or Xij element can be written as identity tensor H transpose acting on X. Where the relation between the X and H, so X and X vector is as follows that if we have let us say X to be x11 x12 x21 x22 just two by two matrix then the vector x will be x11 x12 x21 x22, this is what we have been calling the unfolding of the matrix, so we can relate a matrix with a vector, this is the same vector. Now we go back to our earlier cases that we have H times the rho ij th element and we have rho times H ij th element and that can be written as H rho ij can be written as h tensor identity acting on rho vector and the ij th element of that and rho H ij can be written as identity tensor H transpose acting on rho vector and the ij th element of that.

(Refer slide time: 9:45)



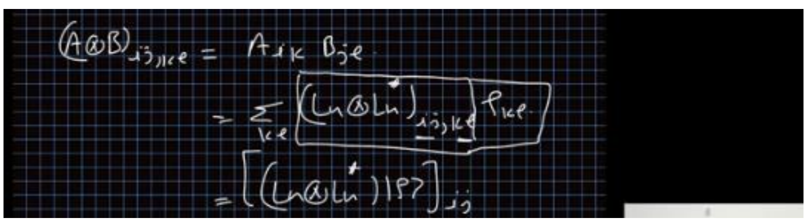
So, this is the first, now the second we have Ln rho Ln dagger and the ij th element of that. That will be Ln ik rho kl Ln dagger lj sum over kl. So, the ij th element of the product of three matrices will be, we take the first two matrix product and the next two matrix product and that's how we get it. So, you see the second index and the first index, they matches and summation over that is there. So, if we just sum over k, we get the product of Ln and rho and the ij th element of that and then the product of that the Ln and rho will be multiplied with Ln dagger, so the second index of the product matches with the first index of the next matrix and we take sum over that, so we are left with i and j element in that way we can take the product of three matrices, and this we can write as sum over kl Ln ik Ln Ln dagger lj rho kl. So rho kl is there, so we can see that there is a index here and there is a k and l index indices are there. so we can see that Ln ik, we can write that as Ln star jl rho kl and if we see that A tensor B ij kl element is A ik B jl. So from here we can see this term can be written as sum over kl Ln tensor Ln star, and that will be ij, kl element and rho kl. Now if we identify ij with one index and kl with another index, then it becomes, this equation will look like as if we have a matrix multiplied with a vector. And we can write it as and the ij element of that will sum over kl. That will be Ln tensor Ln star acting on the vector rho and the element ij.

(Refer slide time: 11:46)



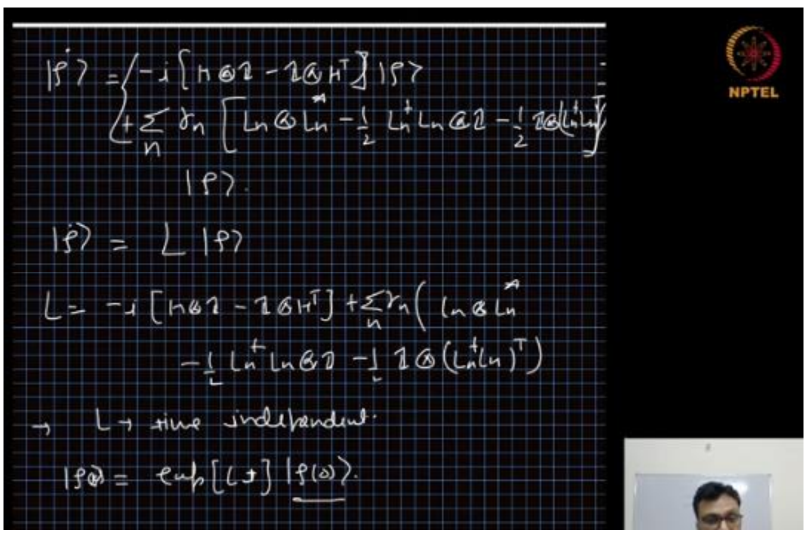
Okay, so what we have done is we have taken Ln rho Ln dagger and the ij th element of that, and that is equivalent to Ln times the Ln star acting on the vector rho the unfolded matrix rho and the ij th element of that. So, with this, we can rewrite the whole master equation as rho ij dot as minus i H tensor identity minus identity tensor H transpose acting on rho and the ij th element of that. So, I'm just removing ij th element because everything is ij th element. So, it will be the vector rho dot equals minus i, H tensor identity minus identity tensor H transpose acting on rho plus the dissipated term, sum over n gamma n, first term was Ln rho Ln dagger which will become Ln tensor Ln star minus 1 over 2. The first term is Ln dagger Ln rho that becomes Ln dagger Ln tensor identity. Second term is rho times Ln dagger Ln, which will be half identity tensor Ln dagger Ln whole transpose.

(Refer slide time: 12:54)



And all these terms are getting multiplied with vector rho. Or we can say there's a matrix L which is acting on rho and we get rho dot equals L rho where L is minus i H tensor identity minus identity tensor H transpose, plus sum over n gamma n and some term which is Ln tensor Ln star minus half Ln dagger Ln tensor identity minus half identity tensor Ln dagger Ln transpose. Now, if L is time independent, If L is time independent, then rho becomes exponential, rho at time t becomes exponential of L t rho at 0. So, it is a simple vector equation now that we have a vector rho and the derivative of vector rho and these two are related by matrix L.

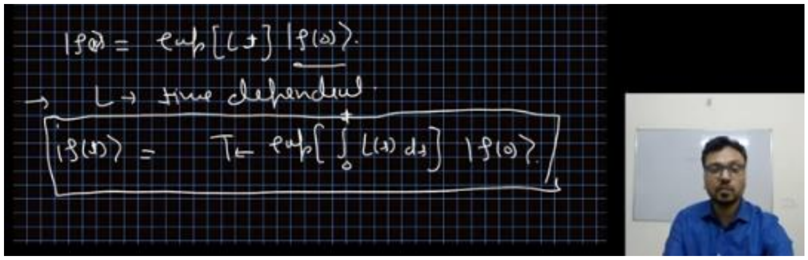
(Refer slide time: 15:30)



So, if L is time independent, then in principle, we can write rho of t equals exponential of L times t acting on rho of 0, that is the state at time t equals 0. And from this, we can calculate the vector rho of 0, we can calculate from the initial state we are given by unfolding the density matrix. And in this way, we can evolve the state and we get a state at time t and then we can fold it back to get the density matrix at time t. If L is time dependent, then the formal solution for rho of t can be written as time ordered operation exponential of 0 to t L of s ds acting on rho of 0. This is the solution when L is time dependent.

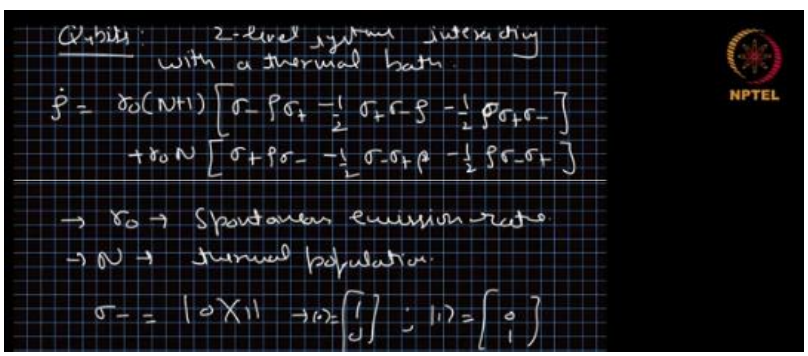
So, in that way, we can formally solve the master equation of any type, the linear master equation. Now, let us take the example of qubits. That is, we have a two-level system interacting with thermal bath. In that case, the density matrix rho dot is given by gamma naught N plus 1. We are just talking about the dissipator.

(Refer slide time: 16:40)



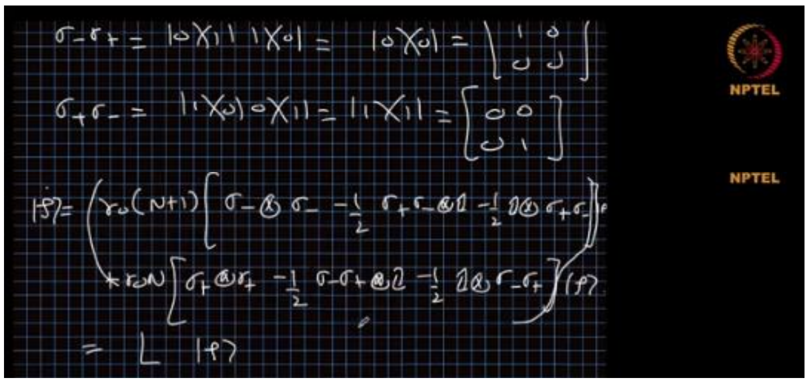
We are not interested in the Hamiltonian dynamics for the Lamb shift. That will be sigma minus rho sigma plus minus half sigma plus sigma minus rho minus half sigma rho sigma plus sigma minus, plus gamma naught times n, sigma plus rho sigma minus, minus half, sigma minus sigma plus rho, minus half rho sigma minus sigma plus. So, this is the Lindblad-Master equation for a two-level system interacting with a thermal bath. Here, gamma naught is the spontaneous emission rate. N is the thermal population.

(Refer slide time: 18:53)



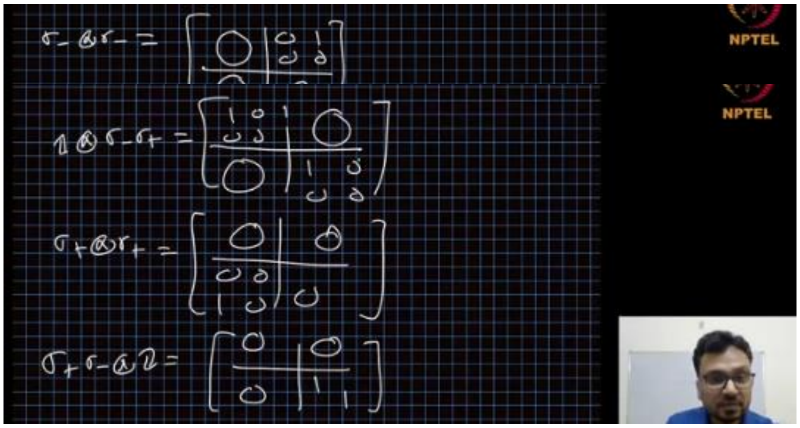
Sigma minus is given by 0 outer product 1, that is if it X on 1 it takes it to 0 and we can write it if 0 is given by and 1 is given by 0 1 then Sigma minus will be 0 1 0 Sigma plus is sigma minus dagger that will be 0 1 0 sigma minus sigma plus will be 0 1 and 1 0 that is just 0 0 this is 1 0 0 0 and sigma plus sigma minus will be 1 0 0 1 which is 1 1, which will be 0001. So, from here, we can see, our rho dot although this was not required at the moment but we can see our rho dot, when we unfolded the vector rho dot can be written as gamma naught N plus 1 sigma minus tensor sigma plus transpose which becomes sigma minus acting on rho vector, minus half sigma plus sigma minus tensor identity minus half identity tensor sigma plus sigma minus transpose, which is again a sigma plus sigma acting on rho vector plus gamma naught N sigma plus tensor sigma plus minus half sigma minus sigma plus tensor identity minus half identity tensor sigma minus sigma acting on rho.

(Refer slide time: 20:47)



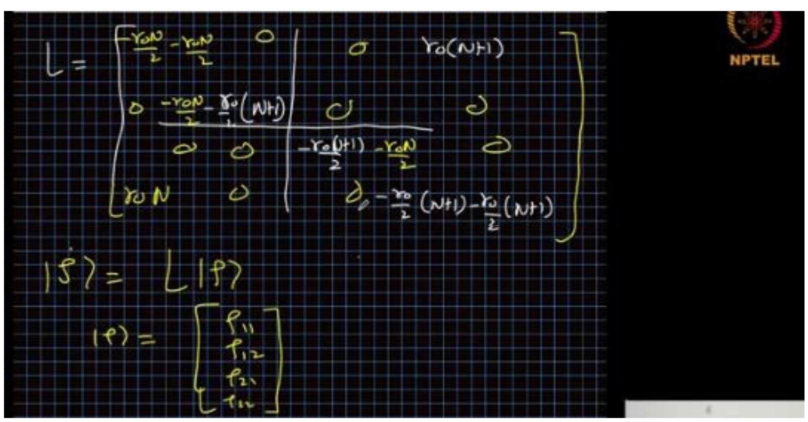
So, this is the equation where we have a matrix L acting on rho where L is given by this whole expression. Now let us calculate L, so for that we see we need sigma minus tensor sigma minus that becomes by looking at the definition of sigma minus it becomes two by two zero two by two zero two by two zero and zero one zero zero. It's a four by four matrix of this form. Sigma plus sigma minus, sigma minus sigma plus is one zero zero zero so this tensor identity one one zero zero zero and identity tensor sigma minus sigma plus will be zero one zero zero zero one zero zero and everything else is zero. Now we substitute or let us calculate others also sigma plus tensor sigma plus will be easy to calculate 0 0 1 0 and everything else is 0. sigma plus sigma minus tensor identity will be Sigma plus sigma minus is this identity will be tensor identity will be just one one zero zero zero it's just opposite of this and identity tensor sigma plus sigma minus will be zero one zero one. I'm sorry this is not correct, It should be sigma minus sigma plus is upper one, so this will be one zero zero zero and this one also one zero zero zero now we have all the operators we wanted so our l becomes make a big matrix here. So, first term is sigma minus times sigma minus with a coefficient gamma naught N plus 1. And the second is minus half times sigma plus sigma minus times identity and minus half times identity times sigma plus sigma minus. So, these two terms we have with minus half times gamma naught N plus 1.

(Refer slide time: 21:43)



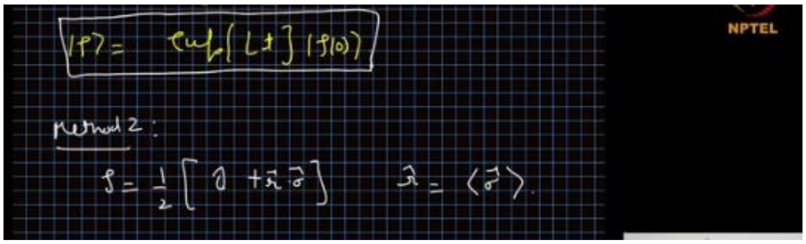
No, no, these two terms, not the first two. So, we are left with minus half gamma naught N plus one and minus half, this is the gamma naught over two N plus one, this comes from this term and from the other term we get minus gamma naught N plus one over two and minus gamma naught over two N plus. This is the contribution from the first big expression in the Lindblad equations. The second will give us the following term.

(Refer slide time: 25:46)



So, it is the sigma plus tensor sigma plus so this is here the element is here and that will be gamma naught times n and we have sigma minus sigma plus tensor identity that will be minus half gamma naught n over 2 and gamma naught N over 2. And we have minus gamma naught N over 2 and minus gamma naught N, so this becomes our element everything else is zero this is zero this is zero zero zero zero zero zero zero zero zero zero now with this we can rewrite the master equation rho dot equals L acting on rho where L is this four by four matrix and rho vector is our rho one one rho one two rho two one rho two, this is our vector and we can now solve it and with this this particular L is the time independent matrix so it becomes our solution becomes exponential of L t the rho of zero. So, this is how we can solve this particular master equation of a two level system interacting with the thermal bath this is one way of solving the master equation there are more than one ways of course the second method to solve master equation is the following. So, let us consider the block representation of the density matrix of a two level system.

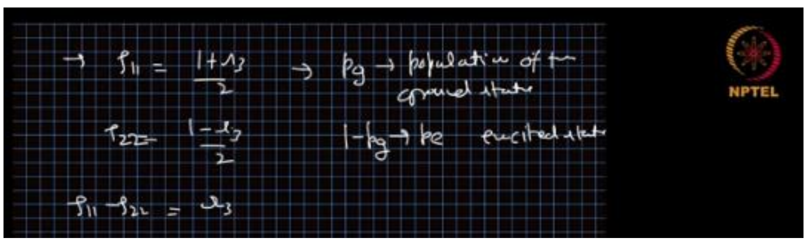
(Refer slide time: 26:40)



So, it is half times identity plus r dot sigma, where r vector is the vector of partition value of sigma matrix. So, our rho can be written as 1 plus r3 over 2 r1 minus i r2 over 2, r1 plus i r2 over 2 and 1 minus r3 over 2. From here we can see rho11 is 1 plus r3 over 2 and that is the population of the ground state. And rho 22, which is 1 minus r3 over 2, that is 1 minus p0 is the population of excited state. g here, the excited state population.

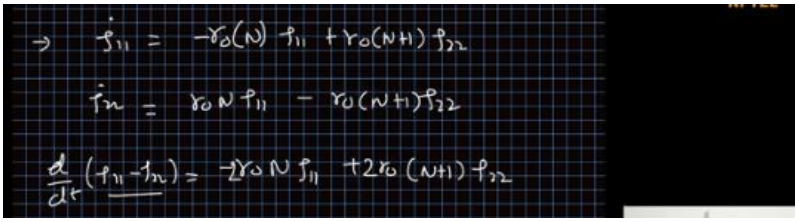
So, these are the populations of the ground and excited state. And from here, we can see rho 11 minus rho 22 will give us. So, from the master equation we just derived for two-level system in terms of L matrices, we can see from this equation, we can see that rho11 dot is gamma naught times N with minus these two. So, minus gamma naught N times rho11 and gamma naught plus gamma naught N plus 1 rho 2 2 and rho 2 2 dot is gamma naught N times rho 1 1 minus gamma naught N plus 1 rho 2 2 so from here here here and here.

(Refer slide time: 27:46)

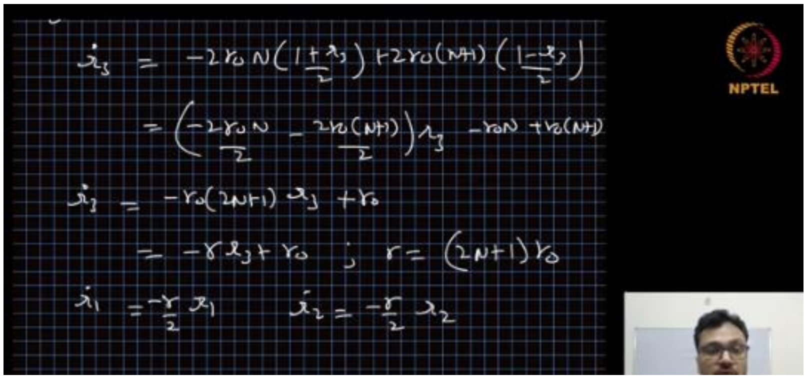


So, from here we can see that rho 1 1 dot and rho 2 2 2 2 dot are closed so rho 1 1 and rho 2 2 are written in terms of rho 1 and rho 2 so if we add if we subtract these two equations we get d over dt of rho 1 1 minus rho 2 2 that will be minus gamma naught N twice rho 1 1 and plus 2 gamma naught N plus 1 rho 2 2 Rho 1 1 minus rho 2 2 is r. So, this is r3. This is r3 dot. We get minus 2 gamma naught N. Rho 1 1 is 1 plus r3 over 2 plus 2 gamma naught N plus 1. That is 1 minus r3 over 2.

(Refer slide time: 29:16)



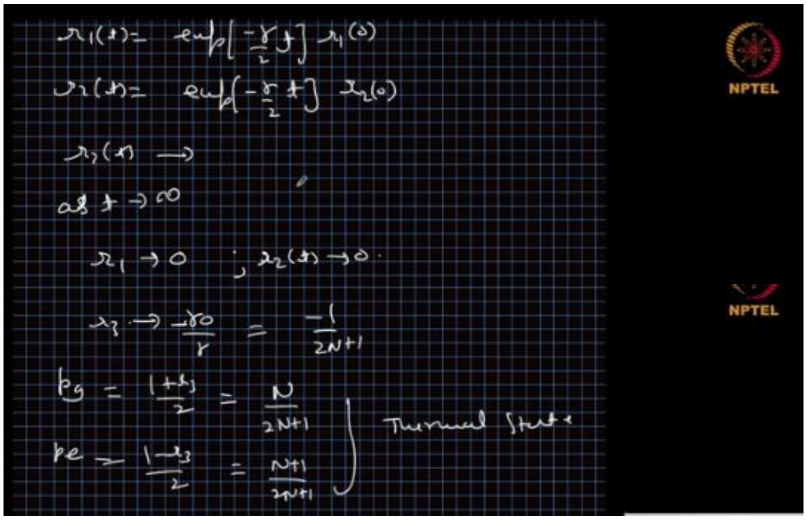
(Refer slide time: 30:57)



From here we can collect the terms which contains r3 and which do not contain r3. So, we get minus 2 gamma naught N over 2 from here and from here we get minus 2 gamma naught N plus 1 over 2 for r3 and we get minus gamma naught N plus gamma naught N plus 1, which are independent of r3. From here we can get minus gamma naught 2N plus 1 r3 plus gamma naught. So, r3 dot is written as minus gamma naught 2N plus 1, r3 plus gamma naught or we can write minus gamma r3 plus gamma naught, where gamma is 2N plus 1 gamma naught. And we can see that r1 dot in the same equation, we can see r1 dot will be r1 dot will be minus gamma over 2 r1 and r2 dot will be minus gamma over 2 r2.

So, from using the Lindblad-Master equation, we have arrived at the equation of the expectation values of the sigma operators or the bloch vector. Here, from here, we can see that r1 of t becomes exponential of minus gamma over 2 t r1 at 0. r2 of t is exponential of minus gamma over 2 t r2 of 0. And we have r3 of t which is some function of t as t tending to infinity the system acquires a steady state and in that we can see that dr over dt should be zero, so r1 goes to zero from this equation you can see when we put t tending to infinity this becomes zero r2 of t tends to 0 because again same equation and r3 of t when t tends to infinity for that we can see that r3 dot will be 0 because it is a steady state, so, there is no change in r3 so when we substitute right hand side to be 0 then r3 becomes gamma naught over gamma with a minus that is minus 1 over 2N plus 1.

(Refer slide time: 32:52)



From here, we can calculate the probability of the ground state and probability of the excited state, which is 1 plus r3 over 2 and 1 minus r3 over 2. And they come out to be N over 2N plus 1, N plus 1 over 2N plus 1. And these are the populations in the thermal state. So, this shows that this particular solution shows that if a two level system is interacting with the thermal bath, the final state of the two level system is also a thermal state. In that way, we have shown that how to solve a master equation and how to arrive at the thermal state, which we did earlier by assuming a thermal state and showing that it is a steady state.